University of Alberta

Superconductivity near boundaries; a wave-function approach

by

Kamran Kaveh-Maryan

A thesis submitted to the Faculty of Graduate Studies and Research in partial fulfillment of the requirements for the degree of Masters of Science

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Abstract

Numerical solutions of the Bogoliubov-De Gennes equations will be investigated for an s-wave superconducting system with boundaries using a tight-binding model. Solutions corresponding to different electron densities and temperatures are presented. Depending on the parameters the Friedel-like oscillations in the gap function are exibited near the boundaries. The qualitative agreement with recent STM experiments is also briefly discussed.

Preface

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Table of Contents

Introduction 1

1 Bogoliubov-de Gennes equations, the mean field formulation for Inhomogeneous Superconductivity 3
- 1.1 How to obtain the Bogoliubov equations: . . . 4
- 1.2 Self-consistency relations . . . 10
- 1.3 Free Energy for an Inhomogeneous Superconductor . . . 13
- 1.4 Homogeneous systems: . . . 14
- 1.5 Perturbation Theory on the BdG equations, the integral equation for the gap function . . . 17
- 1.6 Gor'kov Equations . . . 20

2 Quasi-Classical Approximation 24
- 2.1 Andreev Approximation . . . 24
- 2.2 Analytical Solutions for the Quasi-Classical equation . . . 27
  - 2.2.1 Ansatz Pair-Potentials . . . 29
  - 2.2.2 Exact solutions . . . 29
  - 2.2.3 Requirement of Self-consistency . . . 32
- 2.3 Quasi-Classical equation and Supersymmetric Quantum Mechanics 35

3 Hubbard Model and discretized version of the Bogoliubov-de Gennes equation 38
- 3.1 Introduction . . . 38
- 3.2 Theoretical considerations: . . . 39
  - 3.2.1 Simplified model in the presence of boundaries . . . 42
- 3.3 How the BdG code works: . . . 43
- 3.4 Checking the code with known BCS results . . . 45
- 3.5 Open boundary conditions; deviation from BCS . . . 51
- 3.6 Spatial behaviour of gap function . . . 63
- 3.7 Local Density Of States(LDOS) . . . 73
  - 3.7.1 LDOS in the presence of a single impurity . . . 88

Conclusion **94**

List of Figures

3.1 $\Delta(n_e)$ for $T = 0.01t$ and $|U| = 2.0t$ 48
3.2 $\Delta(n_e)$ for $T = 0.1t$ and $|U| = 2.0t$ 49
3.3 $\Delta(n_e)$ for $T = 0.15t$ and $|U| = 2.0t$ 50
3.4 $\Delta(n_e)$ for PBC, OBC and Imputrity+PBC , $T = 0.01t$ 54
3.5 $\Delta(n_e)$ for PBC, OBC and Imputrity+PBC, $T = 0.1t$ 55
3.6 $\Delta(n_e)$ for PBC and OBC $T = 0.15t$ 56
3.7 $\Delta(n_e)$ for PBC and OBC $T = 0.19t$ 57
3.8 $\Delta(T)$ for $n_e = 0.2$ and $|U| = 2.0t$ 58
3.9 $\Delta(T)$ for $n_e = 0.4$ and $|U| = 2.0t$ 59
3.10 $\Delta(T)$ for $n_e = 0.6$ and $|U| = 2.0t$ 60
3.11 $\Delta(T)$ for $n_e = 0.8$ and $|U| = 2.0t$ 61
3.12 $\Delta(T)$ for $n_e = 1.0$ and $|U| = 2.0t$ 62
3.13 $u_n(x)$ and $v_n(x)$ for $n = 1$ 66
3.14 $u_n(x)$ and $v_n(x)$ for $n = 2$ 67
3.15 Profile of $\Delta(x, T)$ 68
3.16 $\Delta(x)$; $|U| = 0.5t$ near the boundary 69
3.17 $\Delta(x)$ for OBC and PBC + Impurity 70
3.18 $\Delta(x, T)$ for $|U| = 2.0t$ and $N = 32$ 71
3.19 $\Delta(x, n_e)$ for $|U| = 2.0t$ and $N = 32$ 72
3.20 LDOS for $n_e = 1$, $|U| = 2.0t$ and $T = 0.01t$; 1st and 2nd sites . . . 76
3.21 LDOS for $n_e = 1.0$, $|U| = 2.0t$ and $T = 0.01t$; 3rd and 4th sites . . 77
3.22 LDOS for $n_e = 1.0$, $|U| = 2.0t$ and $T = 0.01t$; 50th and 60th sites 78
3.23 LDOS for $n_e = 1.0$, $|U| = 2.0t$ and $T = 0.01t$; 128th and 129th sites 79
3.24 LDOS for $n_e = 1.8$, $|U| = 2.0t$ and $T = 0.01t$; 1st and 2nd sites . . 80
3.25 LDOS for $n_e = 1.8$, $|U| = 2.0t$ and $T = 0.01t$; 3rd and 4th sites . . 81
3.26 LDOS for $n_e = 1.8$, $|U| = 2.0t$ and $T = 0.01t$; 50th and 60th sites 82
3.27 LDOS for $n_e = 1.8$, $|U| = 2.0t$ and $T = 0.01t$; 128th and 129th sites 83
3.28 LDOS for $n_e = 1.0$, $|U| = 2.0t$ and $T = 0.1t$; 1st and 2nd sites . . 84
3.29 LDOS for $n_e = 1.0$, $|U| = 2.0t$ and $T = 0.1t$; 3rd and 4th sites . . 85
3.30 LDOS for $n_e = 1.0$, $|U| = 2.0t$ and $T = 0.1t$; 50th and 60th sites . 86
3.31 LDOS for $n_e = 1.0$, $|U| = 2.0t$ and $T = 0.1t$; 128th and 129th sites 87
3.32 LDOS for $n_e = 1.0$, $|U| = 4.0t$ and $T = 0.01t$; 1st and 2nd sites . . 90

3.33 LDOS for $n_e = 1.0$, $|U| = 6.0t$ and $T = 0.01t$; 1st and 2nd sites . . 91
3.34 LDOS for $n_e = 1.0$, $|U| = 4.0t$ and $T = 0.01t$; 1st and 2nd sites . . 92
3.35 LDOS for $n_e = 1.0$, $|U| = 4.0t$ and $T = 0.01t$; 1st and 2nd sites . . 93

Introduction

The theory of inhomogeneous superconductors is a fairly old subject of study, almost the same age as the microscopic theory of BCS. It first began with Landau-Ginzburg(LG) phenomenological theory, which was successful to explain some inhomogeneity effects in superconductors such as vortices (i.e., Abrikosov solutions of LG) [1] [2]. However, LG theory does not provide a microscopic treatment of superconducting behavior in the presence of inhomogeneities such as: vortices, boundaries and impurities.

The pioneering work based on a mean field Hartree-Fock approximation of Heisenberg field equations was done by Bogoliubov [3] and with a Green's function approach by Gor'kov [4]. They provide a good framework for dealing with Hamiltonians that break BCS translational invariance, but the resulting equations, known as Bogoliubov-de Gennes(BdG) equations (and Gor'kov equations) are quite complicated and should be solved self-consistently to obtain physical results. Because of these problems a self-consistent treatment of the problem was missing till recently. Now with the help of faster computers we are able to solve BdG (or Gor'kov) equations self-consistently. The amount of work being done on a variety of subjects using BdG equations is increasing quickly. For a detailed list of references about the work done in the frame work of the Bogoliubov-de Gennes equation on inhomogeneous superconductors, the reader is referred to [5].

Much of the BdG literature in the past three decades has utilized approximate

semi-analytic solutions. There has remained a lack of more reliable results (i.e., self-consistent solutions). In this thesis I have solved the self-consistent BdG equations in the presence of simple but realistic boundary conditions, based on the tight-binding attractive Hubbard model.

The thesis is divided as follows: after a somewhat brief review of the literature on inhomogeneous superconductivity, based on the Bogoliubov-de Gennes equations, we present new solutions of the BdG equations near boundaries and investigate the different regimes of solutions, changing parameters such as pairing strength, electron density and temperature. With respect to the new STM experiment connected with a non-magnetic impurity on the boundary, we also try to analyze this situation and compare it with the solutions with open boundary conditions. The results are in qualitative agreement with the previous work on solutions of the Gor'kov equation in a continuum [6] and with the STM experiments [7] [8].

Chapter 1

Bogoliubov-de Gennes equations, the mean field formulation for Inhomogeneous Superconductivity

One can imagine that we can generalize the same procedure of the translational invariant BCS (homogeneous systems) theory to an inhomogeneous system. To fulfill this we should adopt the following steps [9]:

- find the wave-function of the one-electron Hamiltonian (including all the inhomogeneity effects) which are solutions of:

$$\varepsilon_n \phi_n = \left(\frac{-\hbar^2(\nabla - ie\mathbf{A}/c)^2}{2m} + U^{(1)}(\mathbf{r}) - \mu\right)\phi_n \tag{1.1}$$

  where ε_n means energy spectrum in the absence of superconductivity $U^{(1)}$ is the external (lattice) potential, μ is the chemical potential and $\mathbf{A}$ is the vector potential.

- Notice that there exist at least two solutions for each energy ε_n: (ε_n is measured relative to Fermi energy.)

$$\phi_n = \phi_n(\mathbf{r})\chi_\uparrow \tag{1.2}$$

and

$$\phi_{\bar{n}} = \phi_n^*(\mathbf{r})\chi_\downarrow \tag{1.3}$$

where $\chi_\uparrow$ or $\chi_\downarrow$ denote the spin states.

- construct a trial function of the BCS type describing a pairing of electrons in the degenerate energy states ϕ_n and $\phi_{\bar{n}}$:

$$\tilde{\Phi} = \prod_n (u_n + v_n a_n^\dagger a_{\bar{n}}^\dagger)\Phi_0 \tag{1.4}$$

where $a_{\bar{n}}^\dagger$ is the creation operator for an electron in the state $\phi_{\bar{n}}$.

In fact, this method has some defects; first is that it is very difficult to solve for ϕ_n's, especially in the presence of some arbitrary geometries, versus in the BCS case where we could assume that $\phi_k(\mathbf{r}) \propto exp(i\mathbf{k}\cdot\mathbf{r})$. In the problems with boundaries ϕ_n will be a stationary wave rather than a plane wave. Also the other problem with this approach is that the energy can often be lowered if we pair the electrons in states that are better choices than ϕ_n.

It was suggested by Bogoliubov [3] that if we *assume* that we have pairing (i.e. superconductivity) with a generalization of Hartree-Fock equations to the case of superconductivity we will get a very practical method to deal with inhomogeneous cases.

1.1 How to obtain the Bogoliubov equations:

We write the Hamiltonian of the system in the second-quantized form as

$$\hat{H} = \hat{H}^{(1)} + \hat{V}^{(2)} \tag{1.5}$$

where $\hat{H}^{(1)}$ is the one-electron (electron-lattice and/or electron-external field) Hamiltonian

$$\hat{H}^{(1)} = \int d^3r \psi^\dagger_\alpha(\mathbf{r})[\frac{-\hbar^2}{2m}(\nabla - ie\mathbf{A}/c)^2\delta_{\alpha\beta} + U^{(1)}_{\alpha\beta}(\mathbf{r})]\psi_\beta(\mathbf{r}) \tag{1.6}$$

while,

$$\hat{V}^{(2)} = -\frac{1}{2}\int d^3r \int d^3r' \psi^\dagger_\delta(\mathbf{r})\psi^\dagger_\gamma(\mathbf{r}')U^{(2)}_{\delta\gamma,\alpha\beta}\psi_\alpha(\mathbf{r}')\psi_\beta(\mathbf{r}) \tag{1.7}$$

is the electron-electron interaction. For simplicity, this potential has been assumed to be time independent (not-retarded); Greek letters denote spin indices and the summation convention is implied. We now assume the simple spin dependence of the interaction,

$$U^{(1)}_{\alpha\beta}(\mathbf{r}) = U^{(1)}(\mathbf{r})\delta_{\alpha\beta} \tag{1.8}$$

$$U^{(2)}_{\delta\gamma\alpha\beta}(\mathbf{r},\mathbf{r}') = U^{(2)}(\mathbf{r},\mathbf{r}')\delta_{\alpha\gamma}\delta_{\delta\beta}. \tag{1.9}$$

Here $\psi_\alpha(\mathbf{r})$ is the usual field operator which destroys a particle of spin α at the point $\mathbf{r}$, and $\psi^\dagger_\alpha(\mathbf{r})$ is the usual field operator which creates a particle of spin α at the point $\mathbf{r}$. They obey the Fermi anti-commutation relations:

$$\psi_\alpha(\mathbf{r})\psi_\beta(\mathbf{r}') + \psi_\beta(\mathbf{r}')\psi_\alpha(\mathbf{r}) = 0 \tag{1.10}$$

$$\psi^\dagger_\alpha(\mathbf{r})\psi_\beta(\mathbf{r}') + \psi_\beta(\mathbf{r}')\psi^\dagger_\alpha(\mathbf{r}) = \delta_{\alpha\beta}\delta(\mathbf{r}-\mathbf{r}'). \tag{1.11}$$

As suggested by Gor'kov [4], we shall assume a contact form for the electron-electron interaction, namely

$$U^{(2)}(r,r') = -g\delta(\mathbf{r}-\mathbf{r}') \tag{1.12}$$

where in an inhomogeneous system, $g = g(\mathbf{r})$. The justification for such a simplification is that the velocity at the Fermi surface (the Fermi velocity) is large compared to the phonon velocity: a virtual phonon is emitted by an electron at some position and does not move much until it is picked up some time later by another electron. The repulsive Coulomb interaction between the electrons is shielded and, therefore, also practically point-like. [1]

Now, defining the Grand-canonical Hamiltonian as

$$\hat{H}' \equiv \hat{H} - \mu\hat{N} \tag{1.13}$$

where $\hat{N} = \int d^3r\psi_\alpha^\dagger(\mathbf{r})\psi_\alpha(\mathbf{r})$ is the number operator , and μ is the chemical potential (for the rest of the thesis we will use prime to show grand canonical hamiltonians). In the self-consistent field approach one seeks an approximate solution of the many-body problem in terms of an effective one-electron Hamiltonian: the best such Hamiltonian of a given form is taken to be the one which minimizes the total free energy. We write this effective Hamiltonian as

$$\hat{H}_{eff} = \int d^3r[\psi_\alpha^\dagger(\mathbf{r})(\mathcal{H}_0 + U(\mathbf{r}))\psi_\alpha(\mathbf{r}) + \Delta(\mathbf{r})\psi_\uparrow^\dagger(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r}) + \Delta^*(\mathbf{r})\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}) + \frac{|\Delta(\mathbf{r})|^2}{g}] \tag{1.14}$$

where

$$\mathcal{H}_0 = \frac{-\hbar^2}{2m}(\nabla - ie\mathbf{A}/c)^2 - \mu.$$

[1] Note that this argument only works for the repulsive interaction, and is not appropriate for the extension of this formalism for attractive Hubbard model hamiltonian.

$U(\mathbf{r})$ is the *mean* (one-electron) potential and $\Delta(\mathbf{r})$ is often referred to as the "pairing potential".[2]

The key feature of the mean-field theory of superconductivity is that we admit non-vanishing expectation values for the spin-paired operators $< \psi_\uparrow^\dagger \psi_\downarrow^\dagger >$ and $< \psi_\downarrow \psi_\uparrow >$. Such expectation values originate from the number non-conserving BCS variational wave function and related ensembles and are referred to as pairing amplitudes. [3]In a non-superconductor, the ψ operators can be expanded in terms of a complete set of wave functions, such as the eigenfunctions ϕ_k of $\mathcal{H}_0$: $\mathcal{H}_0\phi_k = \varepsilon_k\phi_k$ where ε_k are the associated energies (measured from the Fermi energy). Thus, we would write

$$\psi_\alpha(\mathbf{r}) = \sum_k \phi_k(\mathbf{r}) a_{k\alpha} \tag{1.15}$$

where $a_{k\alpha}$ destroys a particle of spin α in state k.[4] In a uniform superconductor, the Hamiltonian (1.14) is diagonalized by a Bogoliubov-Valatin transformation [3]

$$\begin{aligned} a_{k\uparrow} &= U_k \gamma_{k\uparrow} - V_k^* \gamma_{n\downarrow}^\dagger \\ a_{k\downarrow} &= V_k \gamma_{k\downarrow} + U_k^* \gamma_{k\downarrow}^\dagger \end{aligned} \tag{1.16}$$

where $|U_k|^2 + |V_k|^2 = 1$ ensures that if the $a_{k\alpha}$ obey the Fermi anti-commutation rules, then the $\gamma_{k\alpha}$ also will. These anti-commutation rules are

$$a_{k\alpha}a_{k'\beta} + a_{k'\beta}a_{k\alpha} = 0 \tag{1.17}$$

---

[2]The reader should notice the difference between $U^{(1)}(\mathbf{r})$ (lattice potential) and $U(\mathbf{r})$ (Hartree potential), also note that μ appears in $\mathcal{H}_0$ since we want to compare H_{eff} with grand-canonical hamiltonian, H'.

[3]That is why it is difficult to formulate Bogoliubov-de Gennes equations for systems with constant number of electrons (canonical systems) since then, $< \psi\psi >$ and $< \psi^\dagger\psi^\dagger >$ vanish.

[4]From BCS theory we know that the quantum number k is the momentum of the electrons in the condensate.

$$a_{k\alpha}a^{\dagger}_{k'\beta} + a^{\dagger}_{k'\beta}a_{k\alpha} = \delta_{kk'}\delta_{\alpha\beta} \tag{1.18}$$

and

$$\gamma_{k\alpha}\gamma_{k'\beta} + \gamma_{k'\beta}\gamma_{k\alpha} = 0 \tag{1.19}$$

$$\gamma_{k\alpha}\gamma^{\dagger}_{k'\beta} + \gamma^{\dagger}_{k'\beta}\gamma_{k\alpha} = \delta_{kk'}\delta_{\alpha\beta}. \tag{1.20}$$

For a non-uniform superconductor, rather than simply inserting equations (1.16) into equation (1.15) for the two spin states, we seek a more general transformation where *two* sets of eigenfunctions $u_n(\mathbf{r})$ and $v_n(\mathbf{r})$ are introduced and we write ψ_α as

$$\begin{aligned}\psi_\uparrow(\mathbf{r}) &= \sum_n [u_n(\mathbf{r})\gamma_{n\uparrow} - v^*_n(\mathbf{r})\gamma^{\dagger}_{n\downarrow}] \\ \psi_\downarrow(\mathbf{r}) &= \sum_n [u_n(\mathbf{r})\gamma_{n\downarrow} + v^*_n(\mathbf{r})\gamma^{\dagger}_{n\uparrow}].\end{aligned} \tag{1.21}$$

Note that in contrast to (1.16), here all the elementary excitations contribute to the sum since the field operators ψ are basically labeled with spatial coordinates rather than momentum(BCS). In order to satisfy equations (1.10) and (1.11), u_n and v_n must satisfy the normalization and completeness conditions:

$$\int [u^*_n(\mathbf{r})u_m(\mathbf{r}) + v^*_n(\mathbf{r})v_m(\mathbf{r})]d^3\mathbf{r} = \delta_{nm} \tag{1.22}$$

and

$$\sum_n [u^*_n(\mathbf{r})u_n(\mathbf{r}') + v^*_n(\mathbf{r})v_n(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}') \tag{1.23}$$

where $u_n(\mathbf{r})$ and $v_n(\mathbf{r})$ are Bogoliubov (quasi-particle/quasi-hole) amplitudes, and display the amount of contribution of quasi-particles($\gamma^{\dagger}$) or quasi-holes(γ) to the real space operators, $\psi(\mathbf{r})$.

The greater flexibility afforded by equation (1.21) can, in some cases, lead to a lower free energy, assuring a more accurate solution.

We demand that equation (1.21), using (1.22) and (1.23), diagonalize $\hat{H}_{eff}$, i.e.,

$$\hat{H}_{eff} = E_g + \sum_{n\alpha} E_n \gamma^\dagger_{n\alpha} \gamma_{n\alpha} \tag{1.24}$$

where E_g is the ground-state energy. From equations (1.24), (1.19) and (1.20), we have

$$\begin{aligned} \left[\hat{H}_{eff}, \gamma_{n\alpha}\right] &= -E_n \gamma_{n\alpha} \\ \left[\hat{H}_{eff}, \gamma^\dagger_{n\alpha}\right] &= E_n \gamma^\dagger_{n\alpha}. \end{aligned} \tag{1.25}$$

Our strategy will be to evaluate the commutator of $\hat{H}_{eff}$ with $\psi_\uparrow$ and $\psi_\downarrow$ in two non-equivalent ways. For the first of these, we use equations (1.21) and (1.14) to obtain

$$\begin{aligned} \left[\hat{H}_{eff}, \psi_\uparrow(\mathbf{r})\right] &= -[\mathcal{H}_0 + U(\mathbf{r})]\psi_\uparrow(\mathbf{r}) - \Delta(\mathbf{r})\psi^\dagger_\downarrow(\mathbf{r}) \\ \left[\hat{H}_{eff}, \psi_\downarrow(\mathbf{r})\right] &= -[\mathcal{H}_0 + U(\mathbf{r})]\psi_\downarrow(\mathbf{r}) + \Delta(\mathbf{r})\psi^\dagger_\uparrow(\mathbf{r}) \end{aligned} \tag{1.26}$$

after which we insert equation(1.21) into the right hand side. The second way to evaluate the commutator is to substitute equation (1.21) directly, and to evaluate the resulting commutator of the γ operators using equations (1.25). Comparing the coefficients of the γ operators in the two sets of expressions so formed, we obtain Bogoliubov-de Gennes equations:

$$\begin{aligned} E_n u_n(\mathbf{r}) &= [\mathcal{H}_0 + U(\mathbf{r})]u_n(\mathbf{r}) + \Delta(\mathbf{r})v_n(\mathbf{r}) \\ E_n v_n(\mathbf{r}) &= -[\mathcal{H}_0^* + U(\mathbf{r})]v_n(\mathbf{r}) + \Delta^*(\mathbf{r})u_n(\mathbf{r}) \end{aligned} \tag{1.27}$$

which can be written in the matrix form,

$$\hat{H}_{BdG}\begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix} = E_n \begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix} \tag{1.28}$$

where

$$\hat{H}_{BdG} = \begin{pmatrix} \mathcal{H}_0 + U(\mathbf{r}) & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -\mathcal{H}_0^* - U(\mathbf{r}) \end{pmatrix}. \tag{1.29}$$

Note that in a magnetic field the kinetic energy operator $-(\hbar^2/2m)[\nabla-(ie/\hbar c)A]^2$ contains an imaginary cross-term which changes sign on taking the complex conjugate; hence, $\mathcal{H}_0^* \neq \mathcal{H}_0$.

1.2 Self-consistency relations

We must now determine $U(\mathbf{r})$ and $\Delta(\mathbf{r})$ which enter $\hat{H}_{eff}$ from the requirement that the free energy evaluated with the full Hamiltonian, $\hat{H}'$ (defined by the equations (1.5)-(1.13)) be stationary with respect to our chosen expansion of the ψ operators. The free energy is given by

$$\mathcal{F} = < \hat{H}' > - TS \tag{1.30}$$

where the angular brackets imply a combined quantum-mechanical and statistical average, to be performed with a Gibbs ensemble involving the eigenvalues and eigenfunctions of $\hat{H}_{eff}$.

In calculating $\hat{H}'$ we must evaluate a term involving ψ operators occurring in $\hat{V}^{(2)}$. This is most easily accomplished using Wick's theorem which tells us we must form all non-equivalent pairs of ψ operators, with the sign changing every time a pair of operators is commuted. Using this theorem, we have

$$\begin{aligned} < \psi_\alpha^\dagger(\mathbf{r}_1)\psi_\beta^\dagger(\mathbf{r}_2)\psi_\gamma(\mathbf{r}_3)\psi_\delta(\mathbf{r}_4) > \quad &= < \psi_\alpha^\dagger(\mathbf{r}_1)\psi_\beta^\dagger(\mathbf{r}_2) >< \psi_\gamma(\mathbf{r}_3)\psi_\delta(\mathbf{r}_4) > \\ &- < \psi_\alpha^\dagger(\mathbf{r}_1)\psi_\gamma(\mathbf{r}_3) >< \psi_\beta^\dagger(\mathbf{r}_2)\psi_\delta(\mathbf{r}_4) > \\ &+ < \psi_\alpha^\dagger(\mathbf{r}_1)\psi_\delta(\mathbf{r}_4) >< \psi_\beta^\dagger(\mathbf{r}_2)\psi_\gamma(\mathbf{r}_3) > \end{aligned} \tag{1.31}$$

For the case of the simplified spin dependent contact interaction, described by equations (1.8) (1.9) and (1.12), we can write the variation in the free energy as

$$\begin{aligned}\delta\mathcal{F} = \int d^3\mathbf{r} \sum_{\alpha} \{\delta < \psi_\alpha^\dagger(\mathbf{r})\mathcal{H}_0\psi_\alpha(\mathbf{r}) > \; &+ \textstyle\sum_{\alpha,\beta} g < \psi_\alpha^\dagger(\mathbf{r})\psi_\alpha(\mathbf{r}) > \delta < \psi_\beta^\dagger(\mathbf{r})\psi_\beta(\mathbf{r}) > \\ &- g < \psi_\alpha^\dagger(\mathbf{r})\psi_\beta(\mathbf{r}) > \delta < \psi_\beta^\dagger(\mathbf{r})\psi_\alpha(\mathbf{r}) > \\ &+ g < \psi_\uparrow^\dagger(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r}) > \delta < \psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}) > \\ &- g < \psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}) > \delta < \psi_\uparrow^\dagger(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r}) > \} \\ &- T\delta S = 0. \end{aligned} \tag{1.32}$$

Terms of the form $< \psi_\uparrow^\dagger(\mathbf{r})\psi_\downarrow(\mathbf{r}) >$ have been neglected in equation (1.32) since they are non-zero only in a magnetic system (for instance one containing paramagnetic impurities [37]).

Now the free energy formed from our *effective* Hamiltonian and given by

$$\mathcal{F}' \equiv < \hat{H}_{eff} > - TS \tag{1.33}$$

is automatically stationary since our expectation value can be directly expressed (assuming that we know the mean potentials) in terms of the eigenvalues and eigenfunctions of $\hat{H}_{eff}$, i.e., $\delta < \hat{H}_{eff} > - T\delta S = 0$. Using equation(1.14), we have

$$\begin{aligned}\int d^3r \{\delta < \psi_\alpha^\dagger(\mathbf{r}) \left[\mathcal{H}_0 + U(\mathbf{r})\right] \psi_\alpha(\mathbf{r}) > + \Delta(\mathbf{r})\delta < \psi_\uparrow^\dagger(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r}) > \\ + \Delta^*(\mathbf{r})\delta < \psi_\uparrow(\mathbf{r})\psi_\downarrow(\mathbf{r}) > - T\delta S = 0. \end{aligned} \tag{1.34}$$

Comparing equations (1.32) and (1.34), we see that they are the same *provided* that we define the self-consistent potentials $U(\mathbf{r})$ and $\Delta(\mathbf{r})$ according to

$$\begin{aligned} U(\mathbf{r}) &= -g < \psi_\uparrow^\dagger(\mathbf{r})\psi_\uparrow(\mathbf{r}) > = -g < \psi_\downarrow^\dagger(\mathbf{r})\psi_\downarrow(\mathbf{r}) > \\ \Delta(\mathbf{r}) &= g < \psi_\uparrow(\mathbf{r})\psi_\downarrow(\mathbf{r}) > = -g < \psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}) > \end{aligned} \tag{1.35}$$

At this point, we substitute equations (1.21) into equations (1.35). The mean value of the γ operators that then occur are evaluated using the standard rules

$$< \gamma^{\dagger}_{n\alpha}\gamma_{m\beta} >= \delta_{\alpha\beta}\delta_{mn}f_n \tag{1.36}$$

and

$$< \gamma_{n\alpha}\gamma_{m\beta} >= 0. \tag{1.37}$$

Here

$$f_n = \frac{1}{\exp(\beta E_n) + 1} \tag{1.38}$$

is the usual Fermi occupation factor. Performing these calculations, we have

$$\begin{aligned} U(\mathbf{r}) &= g\sum_n \{|u_n(\mathbf{r})|^2 f_n + |v_n(\mathbf{r})|^2(1-f_n)\} \\ \Delta(\mathbf{r}) &= -g\sum_n v_n^*(\mathbf{r})u_n(\mathbf{r})(1-2f_n). \end{aligned} \tag{1.39}$$

We see that the superconductivity in an inhomogeneous system is governed by a system of equations involving the Bogoliubov-de Gennes equations (1.27), and two self-consistency conditions, equations (1.39).

In practice there is an important distinction between $U(\mathbf{r})$ and $\Delta(\mathbf{r})$. The Hartree-Fock potential $U(\mathbf{r})$ comes from an integral $\sum_n$ involving all states below the Fermi level. Consequently, $U(\mathbf{r})$ is nearly independent of temperature, and U can be approximated by the Hartree-Fock potential calculated *in the normal state.* This represents a considerable simplification. On the contrary, the pair potential $\Delta(\mathbf{r})$ is a sum of terms of form $u_n v_n^*$. Such a term is nonzero only in the neighborhood of the Fermi surface. For this reason $\Delta(\mathbf{r})$ is a strong function of temperature.

1.3 Free Energy for an Inhomogeneous Superconductor

We begin with the density matrix obtained from $\hat{H}_{eff}$:

$$\hat{\rho} = \frac{\exp(-\beta \hat{H}_{eff})}{Tr\{\exp(-\beta \hat{H}_{eff})\}}. \tag{1.40}$$

It is also known that the entropy of an ideal gas of fermionic (quasi-) particles, can be expressed in terms of the mean occupation numbers f_n as [35]

$$S = 2\sum_n \{f_n \ln f_n + (1 - f_n)\ln(1 - f_n)\} \tag{1.41}$$

where the factor of two accounts for the two independent spin orientations. Thus, inserting equations (1.24), (1.36) and (1.41) into the definition of free energy, which is a functional of the pair-potential and the mean occupation number f_n, it can be written as

$$\mathcal{F} = \mathcal{F}[\Delta(\mathbf{r}), f_n] = E_g + 2\sum_n E_n f_n - 2k_B T \sum_n \{f_n \ln f_n + (1 - f_n)\ln(1 - f_n)\}. \tag{1.42}$$

The expression of the free energy can be further simplified. Inserting (1.38) into (1.42) yields after some straightforward algebra

$$\mathcal{F} = -2k_B T \sum_n \ln\left(2\cosh(\beta E_n)\right) + \int d^3r \frac{|\Delta(\mathbf{r})|^2}{g} \tag{1.43}$$

where the term $|\Delta(\mathbf{r})|^2$ is the contribution of the ground-state energy.

Apparently, in order to calculate the free energy (1.43), it is necessary to know the spectrum $\{E_n\}$ of the BdG operator, H_{BdG}, for a given pair-potential $\Delta(\mathbf{r})$ (and boundary condition). Fortunately, this is not the case as several authors have already shown [14] [36], albeit in the absence of a magnetic field. Indeed, by employing the identity

$$\cosh^2\left(\frac{x}{2}\right) = \prod_{m=0}^{\infty}\left[1+\frac{x^2}{\pi^2(2m+1)^2}\right] \tag{1.44}$$

the free energy (1.43) can be recast as

$$\mathcal{F} = -2k_BT\sum_i \ln\left(2\prod_{\omega_m>0}\frac{\omega_m^2+E_i^2}{\omega_m^2}\right) + \int d^3\mathbf{r}\frac{|\Delta(\mathbf{r})|^2}{g} \tag{1.45}$$

where $\omega_m = \pi k_BT(2m-1)$ are fermionic Matsubara frequencies. The divergence of the above expression for the free energy (in inifinite systems) can be eliminated by subtracting from $\mathcal{F}$ (i.e., by measuring $\mathcal{F}$ with respect to) the free energy of the corresponding normal state, Thus, by denoting $\delta\mathcal{F} \equiv \mathcal{F} - \mathcal{F}_N$ we have

$$\begin{aligned}\delta\mathcal{F} &= -2k_BT\sum_i \ln\left(2\prod_{\omega_m>0}\frac{\omega_m^2+E_i^2}{\omega_m^2+\varepsilon_i^2}\right) + \int d^3r\frac{|\Delta(\mathbf{r})|^2}{g} \\ &= -2k_BT\sum_{\omega_m>0}\ln\left(Det\left(\frac{\omega_m^2+\hat{\mathcal{H}}_{BdG}^2}{\omega_m^2+\hat{H}_0^2}\right)\right) + \int d^3\mathbf{r}\frac{|\Delta(\mathbf{r})|^2}{g}\end{aligned} \tag{1.46}$$

where H_0 is the BdG Hamiltonian corresponding to the normal state of the system (i.e., $\Delta \equiv 0$),and $\{\varepsilon_i\}$ denotes the spectrum of H_0[5].

1.4 Homogeneous systems:

As we should expect, the BCS equations will be recovered as a special case of the BdG equations with $\Delta(\mathbf{r}) = \Delta_0$[6]. This can be easily observed by introducing the Fourier transform of the Bogoliubov amplitudes $u_n(\mathbf{r})$ and $v_n(\mathbf{r})$ as

$$\begin{aligned}u_n(\mathbf{r}) &= \sum_k U_n(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r}) \\ v_n(\mathbf{r}) &= \sum_k V_n(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r})\end{aligned} \tag{1.47}$$

[5]For methods to further simplify the form of the free energy c.f. Eilenberger and Jacobs(1975) and Waxman(1994).

[6]Also. for simplicity, we assume $U(\mathbf{r}) = 0$, but the same results can be derived for the more general situation when $U(\mathbf{r})$ is non-zero.

Inserting these into the BdG equation, we get the equation for U_k and V_k:

$$\begin{aligned}(\varepsilon_k - E_n)U_n(\mathbf{k}) + \Delta_0 V_n(\mathbf{k}) = 0 \\ (-\varepsilon_k - E_n)V_n(\mathbf{k}) + \Delta_0 U_n(\mathbf{k}) = 0\end{aligned} \tag{1.48}$$

This gives us the dispersion relation (i.e., $E_n = E_n(\mathbf{k})$) for every normal mode with momentum $\mathbf{k}$, [7] as it can be seen from equation (1.47) we are basically able to determine energy index, n, from momentum $\mathbf{k}$, so from now on we drop all the quasi-particle energy indices , n. Taking the determinant of equation (1.48) gives the dispersion relation :

$$E_n = \sqrt{\Delta_0^2 + \varepsilon_k^2} \tag{1.49}$$

and the corresponding eigenvectors

$$\begin{aligned}U_k &= \sqrt{\frac{1}{2}(1 + \frac{\varepsilon_k}{E_k})} \\ V_k &= \sqrt{\frac{1}{2}(1 - \frac{\varepsilon_k}{E_k})}.\end{aligned} \tag{1.50}$$

Inserting U_k, V_k and E_k in the self-consistency relations (1.39) also provides us with the BCS *gap equation*

$$\Delta_0 = |g| \sum_k \frac{1}{2} \frac{\Delta_0}{E_k} [1 - 2f(E_k)] \tag{1.51}$$

Another interesting homogeneous case is the state of *uniform flow*, i.e. having a uniform current in the system. In this case the magnitude of the pair-potential is constant but it has a spatially dependent phase:

$$\Delta(\mathbf{r}) = \Delta_0 \exp(2i\mathbf{q} \cdot \mathbf{r}), \tag{1.52}$$

[7] Note that in equation (1.48), ε_k appears since $\mathcal{H}_0 \exp(i\mathbf{k} \cdot \mathbf{r}) = \varepsilon_k \exp(i\mathbf{k} \cdot \mathbf{r})$.

where $\mathbf{q}$ is a vector in the direction of the flow (the average momentum per electron in this state is $\hbar\mathbf{q}$). This form for $\Delta(\mathbf{r})$ can be understood from the Gor'kov derivation of the LG equations as an asymptotic approximation of the BdG (or Gor'kov) equations [10]. He showed that the Landau-Ginzburg order parameter Ψ is proportional to the pair-potential Δ. This fact plus the relation $\mathbf{j} \propto \Psi^*\nabla\Psi - \Psi\nabla\Psi^*$ gives

$$\mathbf{j} \propto \mathbf{q}|\Delta|. \tag{1.53}$$

A useful fact is the *gauge invariance* of the BdG equations (as shown in de Gennes(1966) [9]). Introduction of the phase $\chi(\mathbf{r})$ will give rise to changes in u_n, v_n and Δ as,

$$\begin{aligned} u_n' &= u_n \exp(i\chi(\mathbf{r})) \\ v_n' &= v_n \exp(-i\chi(\mathbf{r})) \\ \Delta' &= \Delta_0 \cdot \exp(2i\chi(\mathbf{r})). \end{aligned} \tag{1.54}$$

Using the form of $2\mathbf{q}\cdot\mathbf{r}$ for $\chi(\mathbf{r})$, we can write u_n and v_n as

$$\begin{aligned} u_n(\mathbf{r}) &= U_k \exp(i(\mathbf{k}+\mathbf{q})\cdot\mathbf{r}) \\ v_n(\mathbf{r}) &= V_k \exp(i(\mathbf{k}-\mathbf{q})\cdot\mathbf{r}) \end{aligned}$$

The rest of the calculations are straightforward and similar to what we did for BCS in the absence of the current. The same procedure will give rise to the BdG equations in the following form:

$$\begin{aligned} (E_k - \varepsilon_{k+q})U_k - \varepsilon_{k-q}V_k &= 0 \\ -\varepsilon_{k+q}U_k + (\varepsilon_k + \varepsilon_{k-q})V_k &= 0 \end{aligned} \tag{1.55}$$

where the positive eigenvalue E_k is given by

$$E_k = \frac{\varepsilon_{k+q} - \varepsilon_{k-q}}{2} + \left[(\frac{\varepsilon_{k+q} - \varepsilon_{k-q}}{2})^2 + |\Delta|^2 \right]^{1/2} \tag{1.56}$$

Since the coherence length ξ_0 in a conventional superconductor is about $\hbar k_F/\Delta_0$, the region of major interest is $q \sim \Delta/\hbar v_F$ and thus $q \ll k_F$. Retaining only terms to first order in q, we can write

$$\frac{\varepsilon_{k+q} - \varepsilon_{k-q}}{2} = \frac{\hbar \mathbf{k} \cdot \mathbf{q}}{m}$$

$$\frac{\varepsilon_{k+q} + \varepsilon_{k-q}}{2} = \varepsilon_k$$

$$E_k = E_k^0 + \frac{\hbar \mathbf{k} \cdot \mathbf{q}}{m}$$

1.5 Perturbation Theory on the BdG equations, the integral equation for the gap function

In the normal state the eigenfunctions follow from the solution of

$$\mathcal{H}_0 \phi_n = \varepsilon_n \phi_n$$

or

$$\varepsilon_n \phi_n = (\frac{-\hbar^2 \nabla^2}{2m} + U_0(\mathbf{r}) - \mu)\phi_n \tag{1.57}$$

Near the superconducting transition, we expect u_n and v_n to differ slightly from ϕ_n and it is natural to seek an approximate solution using perturbation theory. We introduce the expansions

$$u_n = u_n^{(0)} + u_n^{(1)} + u_n^{(2)} + \cdots$$

$$v_n = v_n^{(0)} + v_n^{(1)} + v_n^{(2)} + \cdots$$

$$E_n = \varepsilon_n + \varepsilon_n^{(1)} + \varepsilon_n^{(2)} + \cdots \tag{1.58}$$

where according to our notation, ε_n indicates the energy in the zeroth order on Δ, i.e, normal state.

From the structure of equations (1.27) or (1.28), it is apparent that, when $\Delta = 0$, the solutions are restricted in energy and have the form

$$\begin{aligned} u_n^{(0)} &= \phi_n \theta(\varepsilon_n) \\ v_n^{(0)} &= \phi_n^* \theta(-\varepsilon_n) \end{aligned} \tag{1.59}$$

where $\theta(x)$ is the Heaviside (or step) function. Note that from the equation (1.59) the v_n are eigenfunctions of $\mathcal{H}_0'^* + U$ when $\Delta = 0$ and hence the appropriate eigenfunctions are ϕ_n^* as we have written in equation (1.27) and (1.28).

Since $u_n^{(0)} v_n^{(0)} = 0$ in equation (1.39), Δ vanishes in zero order. We expand $u_n^{(1)}$ and $v_n^{(1)}$ in terms of the complete and orthonormal set ϕ_m:

$$u_n^{(1)} = \sum_m a_{nm}\phi_m, \qquad v_n^{(1)} = \sum_m b_{nm}\phi_m. \tag{1.60}$$

If we insert these expansions into the equations (1.27) and (1.28), multiply the first equation by ϕ_m^* and the second by ϕ_m, and integrate over $\mathbf{r}$ we obtain (for $m \neq n$)

$$\begin{aligned} a_{mn} &= \frac{\theta(-\varepsilon_n)}{|\varepsilon_n| - \varepsilon_m} \int \Delta(\mathbf{r}) \phi_m^*(\mathbf{r}) \phi_n^*(\mathbf{r}) d^3\mathbf{r} \\ b_{mn} &= \frac{\theta(+\varepsilon_n)}{|\varepsilon_n| + \varepsilon_m} \int \Delta^*(\mathbf{r}) \phi_m(\mathbf{r}) \phi_n(\mathbf{r}) d^3\mathbf{r}. \end{aligned} \tag{1.61}$$

Inserting the values of a_{mn} and b_{mn} obtained from equation (1.60) into equation (1.59), and using the resulting $u_n^{(1)}$ and $v_m^{(1)}$ in equation (1.35), we obtain the first order correction to the self-consistency condition for $\Delta(\mathbf{r})$ which is an integral equation of the form

$$\Delta(\mathbf{r}) = \int K(\mathbf{r},\mathbf{r}')\Delta(\mathbf{r}')d^3\mathbf{r}', \tag{1.62}$$

where the kernel is defined as

$$K(\mathbf{r},\mathbf{r}') = |g|\sum_{mn}[1-2f(|\varepsilon_n|)]\left(\frac{\theta(\varepsilon_n)}{|\varepsilon_n|+\varepsilon_m}+\frac{\theta(-\varepsilon_n)}{|\varepsilon_n|-\varepsilon_m}\right)\phi_n^*(\mathbf{r})'\phi_m^*(\mathbf{r}')\phi_n(\mathbf{r})\phi_m(\mathbf{r}). \tag{1.63}$$

This is a very important formula, first introduced by Gor'kov [4] in the framework of Gor'kov equations . We will try to manipulate the sums appearing in the kernel so that we can get a physical result for the solutions of the integral equation that are directly expressible in terms of the kernel [11] [12]. Noting that,

$$\frac{\theta(-\varepsilon_n)}{|\varepsilon_n|-\varepsilon_m} = -\frac{\theta(-\varepsilon_n)}{\varepsilon_n+\varepsilon_m}$$

and using the identity

$$1-2f(\varepsilon_n) = \tanh(\beta\varepsilon_n/2)$$

(and the fact that this function is odd) and symmetrizing the expression with respect to m and n, we may rewrite equation(1.62) as

$$K(\mathbf{r},\mathbf{r}') = \frac{|g|}{2}\sum_{mn}\frac{\tanh(\beta\varepsilon_n/2)+\tanh(\beta\varepsilon_m/2)}{\varepsilon_n+\varepsilon_m}\phi_n^*(\mathbf{r}')\phi_m^*(\mathbf{r}')\phi_n(\mathbf{r})\phi_m(\mathbf{r}) \tag{1.64}$$

We now write equation(1.62) in another form by noting that the function $\tanh(x)$ has poles with a residue at $x = (\nu+\frac{1}{2})i\pi$ where ν is the set of all integers. Using a theorem of complex functions, we may regard $\tanh(x)$ as the analytic continuation of the function

$$\sum_{\nu}\frac{1}{x\pm(\nu+\frac{1}{2})i\pi}$$

or

$$\tanh(\frac{\beta\varepsilon}{2}) = 2k_BT\sum_{\nu}\frac{1}{\varepsilon \pm i\hbar\omega_\nu} \tag{1.65}$$

where $\hbar\omega_\nu \equiv 2\pi k_BT(\nu + \frac{1}{2})$. We may then write

$$\begin{aligned}\frac{\tanh(\beta\varepsilon_n/2) + \tanh(\beta\varepsilon_m/2)}{\varepsilon_n + \varepsilon_m} &= 2k_BT\sum_{\nu}\frac{1}{\varepsilon_n + \varepsilon_m}\left(\frac{1}{\varepsilon_n - i\hbar\omega_\nu} + \frac{1}{\varepsilon_m + i\hbar\omega_\nu}\right) \\ &= 2k_BT\sum_{\nu}\frac{1}{(\varepsilon_n - i\hbar\omega_\nu)(\varepsilon_m + i\hbar\omega_\nu)}\end{aligned} \tag{1.66}$$

Thus

$$\mathbf{K(r,r')} = \mathbf{g(r)k_BT}\sum_{\omega}\frac{\phi_{\mathbf{n}}^{*}(\mathbf{r'})\phi_{\mathbf{m}}^{*}(\mathbf{r'})\phi_{\mathbf{n}}(\mathbf{r})\phi_{\mathbf{m}}(\mathbf{r})}{(\varepsilon_{\mathbf{n}} - \mathbf{i\hbar}\omega)(\varepsilon_{\mathbf{m}} + \mathbf{i\hbar}\omega)}. \tag{1.67}$$

It will turn out to be important to write the energy denominator in equation (1.66) as

$$\frac{1}{(\varepsilon_n - i\hbar\omega_\nu)(\varepsilon_m + i\hbar\omega_\nu)} = \int d\varepsilon d\varepsilon' \frac{\delta(\varepsilon - \varepsilon_n)\delta(\varepsilon' - \varepsilon_n)}{(\varepsilon - i\hbar\omega_\nu)(\varepsilon' + i\hbar\omega_\nu)}. \tag{1.68}$$

From now on, we may proceed to use the quasi-classical approximation to simplify the Kernel more. For details of implementing this semi-classical method to calculate the Kernel, we refer the reader to [12][**22**] [13][21]. For the next chapter we come back to the more fundamental Green's function approach (vs. wave-function approach) that is known as the Gor'kov equations.

1.6 Gor'kov Equations

The Green's function approach to inhomogeneous superconductivity is actually older than the wave-function approach (Bogoliubov-de Gennes equations). Before de-Gennes applied BdG to various cases of inhomogeneous superconductivity problems in which Landau-Ginzburg theory was no longer valid, Gor'kov, by

introducing his own equations, proved that Landau-Ginzburg theory is an expansion (in terms of perturbative parameter $T - T_c$) of the free-energy calculated from the Gor'kov equations and the equivalent approach was done through the BdG equations afterwards.

We define

$$G(\mathbf{r}_1, \mathbf{r}_2, \tau_1, \tau_2) \equiv - < T_\tau \psi_\uparrow(\mathbf{r}_1, \tau_1) \psi_\downarrow^\dagger(\mathbf{r}_2, \tau_2) > \tag{1.69}$$

where $\tau = \mathbf{it}$ and the field operators have been written as $\tau - dependent$ (using the Heisenberg picture). Every operator can be written as

$$A(\tau) = \exp(\tau H'/\hbar) A(0) \exp(-\tau H'/\hbar) \tag{1.70}$$

where H' is the garnd-canonical hamiltonian defined in equation (1.6).

Now, using the Heisenberg equations of motions for ψ and $\psi^\dagger$

$$\begin{aligned} (-\frac{\hbar\partial}{\partial\tau} + \frac{\hbar^2}{2m}\nabla^2 + \mu)\psi_\alpha(\mathbf{r}) - g\sum_\beta \psi_\beta^\dagger(\mathbf{r})\psi_\beta(\mathbf{r})\psi_\alpha(\mathbf{r}) = 0 \\ (-\frac{\hbar\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2 - \mu)\psi_\alpha^\dagger(\mathbf{r}) + g\sum_\beta \psi_\alpha^\dagger(\mathbf{r})\psi_\beta^\dagger(\mathbf{r})\psi_\beta(\mathbf{r}) = 0, \end{aligned} \tag{1.71}$$

the equation of motion for $G(\mathbf{r}, \mathbf{r}')$ becomes:

$$\left[\frac{\hbar\partial}{\partial\tau} + \frac{\hbar^2}{2m}\nabla^2 + \mu\right] G(\mathbf{r}_1, \mathbf{r}_2, \tau_1, \tau_2) - \Delta(\mathbf{r}_1) < T_\tau \psi_\downarrow^\dagger(\mathbf{r}_1, \tau - 1)\psi_\uparrow^\dagger(\mathbf{r}_2, \tau_2) > = \delta(\tau_1 - \tau_2)\delta(\mathbf{r}_1 - \mathbf{r}_2) \tag{1.72}$$

If we introduce a new Green function

$$F^\dagger(\mathbf{r}_1, \mathbf{r}_2, \tau_1, \tau_2) = < T_\tau \psi_\downarrow^\dagger(\mathbf{r}_1, \tau_1)\psi_\uparrow^\dagger(\mathbf{r}_2, \tau_2) > \tag{1.73}$$

we get

$$\left[\frac{\hbar\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2 - \mu\right] G(\mathbf{r}_1, \mathbf{r}_2, \tau_1, \tau_2) - \Delta(\mathbf{r}_1) F^\dagger(\mathbf{r}_1, \mathbf{r}_2, \tau_1, \tau_2) = \delta(\tau_1 - \tau_2)\delta(\mathbf{r}_1 - \mathbf{r}_2). \tag{1.74}$$

In the same way, we get the equation for $F^\dagger(\mathbf{r}_1, \mathbf{r}_2, \tau_1, \tau_2)$ as

$$\left[\frac{\hbar\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2 + \mu\right] F^\dagger(\mathbf{r}_1, \mathbf{r}_2, \tau_1, \tau_2) - \Delta(\mathbf{r}_1) G(\mathbf{r}_1, \mathbf{r}_2, \tau_1, \tau_2) = 0 \tag{1.75}$$

where $\Delta(\mathbf{r})$ in defined the same way as in the BdG case, in terms of Green's functions:

$$\Delta(\mathbf{r}) = |g| F(\mathbf{r}, \mathbf{r}; \tau, \tau) \tag{1.76}$$

The above equations are called *Gor'kov equations.*

In a superconducting state which is in equilibrium, the Green functions depend on the difference $\tau - \tau'$. So we can write the transforms

$$G(\mathbf{r}, \mathbf{r}'; \tau) = \sum_n G(\omega_n; \mathbf{r}, \mathbf{r}') e^{i\omega_n \tau}, \qquad F(\mathbf{r}, \mathbf{r}'; \tau) = \sum_n F(\omega_n; \mathbf{r}, \mathbf{r}') e^{i\omega_n \tau} \tag{1.77}$$

and from equations (1.73) and (1.74), we get

$$[i\hbar\omega - \hat{\tau}_3(\frac{\hbar^2}{2m}\nabla^2 + \mu) - \frac{1}{2}(\Delta(\mathbf{r}_1)\hat{\tau}_+ + \Delta^\dagger(\mathbf{r}_1)\hat{\tau}_-)]\hat{G}(\omega; \mathbf{r}_1, \mathbf{r}_2) = \delta(\mathbf{r}_1 - \mathbf{r}_2) \tag{1.78}$$

where

$$\hat{G}(\omega; \mathbf{r}_1, \mathbf{r}_2) = \left[\begin{pmatrix} G(\omega; \mathbf{r}_1, \mathbf{r}_2) & -F^\dagger(\omega; \mathbf{r}_1, \mathbf{r}_2) \\ -F(\omega; \mathbf{r}_1, \mathbf{r}_2) & G(\omega; \mathbf{r}_1, \mathbf{r}_2) \end{pmatrix}\right] \tag{1.79}$$

and $\hat{\tau}_3, \hat{\tau}_\pm = \hat{\tau}_1 \pm i\hat{\tau}_2$ are matrices in the pseudspin space.

The Gor'kov equations and the Bogoliubov-de Gennes equations are equivalent formalisms in the weak coupling approximation, where there is no time

delay in the interaction. In cases in which an average over impurity positions are involved, however, the Gor'kov equations must be employed since it is not the wave-functions but the Green's functions (the correlation functions) that need to be averaged.

It is difficult to solve the Gor'kov equations in the presence of a magnetic field or in the analysis of the proximity effect, which appears when a superconducting metal is in contact with a normal metal. The crudest approximation which is useful to treat these systems is the Landau-Ginzburg theory which is applicable when the scale of the spatial variation, L , of the system satisfies $L \gg \xi_0$ (where ξ_0 is the LG coherence length). The semi-classical approximation (next chapter) is a useful method when $\xi_0 \geq L \gg k_F^{-1}$. It is assumed there that the amplitude of all the quasi-particle momenta $\mathbf{k}$ is k_F and the energy associated with the spatial variation is approximated by $v_F(\hat{\mathbf{k}} \cdot \nabla)$. Since under this approximation, there will be a lot more freedom to manipulate the BdG equations and get self-consistent analytical results we devote the next chapter to a brief review of this method and its different physical achievements.

Chapter 2

Quasi-Classical Approximation

2.1 Andreev Approximation

Superconductors are characterized by at least two different energy scales, namely the Fermi energy E_F and the amplitude of the pair-potential (gap function) Δ_0 at zero temperature. The length scales corresponding to these energies are the Fermi wave-length, $\lambda_F \sim \hbar v_F/E_F$, which gives the mean inter-particle distance in the system, and the superconducting coherence length , $\xi_0 \sim \hbar v_F/\Delta_0$, which determines the spatial extent of the pair correlation. Since, in conventional superconductors $E_F \gg \Delta_0$ (or $\lambda_F \ll \xi_0$), as long as we are interested only in the low energy (or long wavelength) properties of the system it is legitimate to employ the quasi-classical approximation of the theory of superconductivity. The BdG equations are valid on an atomic scale and therefore the spinor wave-function $(u_n(\mathbf{r}), v_n(\mathbf{r}))$, which varies on a length scale set by k_F^{-1}, contains more information than is necessary to calculate, for example, the free energy and free energy density of an inhomogeneous superconductor. In general, this excess of information is eliminated at the end of the calculations by integrating out the irrelevant high energy (of rapidly oscillating) degrees of freedom. A more practical approach, however, is to eliminate these irrelevant degrees of freedom at the beginning of the calculations by replacing the BdG equations with their

quasi-classical limit as suggested first by Andreev [32]. To implement this approximation we mainly follow the approach by Bardeen [15] which is based on the Hamilton-Jacobi equations of motion in **classical** mechanics .

Condsider the semi-classical solution of

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - \mu + U(\mathbf{r})\right)\left(\mathcal{A}(\mathbf{r})e^{ik_F S(\mathbf{r})/\hbar}\right) = 0 \tag{2.1}$$

where the chemical potential, μ, has the value of about the Fermi energy ($\mu = \hbar^2 k_F/2\mathbf{m}$) and $U_0(\mathbf{r})$ is some external potential (in semi-classical BdG equation it will be the Hartree potential). Both $\mathcal{A}(\mathbf{r})$ and $S(\mathbf{r})$ are taken to be slowly varying (with respect to λ_F). From equation (2.1), the Hamilton-Jacobi equations can be written as: [16]

$$\hbar^{-2}|\nabla S(\mathbf{r})|^2 = 1 - 2mk_F^{-2}U(\mathbf{r} \tag{2.2}$$

and the conservation condition

$$\nabla \cdot \left(\mathcal{A}(\mathbf{r})^2 \nabla S(\mathbf{r})\right) = 0. \tag{2.3}$$

the above Hamilton-Jacobi equations can be easily obtained through the applying the Laplacian on the propsed solution $\mathcal{A}\exp(ik_F S/\hbar)$ and gathering different powers of $\hbar$.

We now use the resulting semi-classical solution, which is specified in terms of incoming momentum orientation $\hat{\mathbf{n}}$ via the asymptotic behavior $S(\mathbf{r};\hat{\mathbf{n}}) \sim \hat{\mathbf{n}}\cdot\mathbf{r}$ for $\mathbf{r}$ far from the scattering center and includes all of the fast (i.e., order of λ_F) variations of the exact eigenfunction, to perform a generalized separation of rapidly and slowly varying components of the BdG solutions by writing

$$\begin{pmatrix} u_n(\mathbf{r}) \\ v_n(\mathbf{r}) \end{pmatrix} = \mathcal{A}(\mathbf{r})e^{ik_F S(\mathbf{r};\hat{\mathbf{n}})/\hbar}\begin{pmatrix} \tilde{u}_n(\mathbf{r}) \\ \tilde{v}_n(\mathbf{r}) \end{pmatrix}. \tag{2.4}$$

where $\bar{u}$ and $\bar{v}$ are assumed to be slowly varying relative to λ_F. Now the effect of $\mathcal{H} \equiv \mathcal{H}_0 + U(\mathbf{r})$ in equations (1.27) and (1.28) can be written as:

$$[\mathcal{H}(\mathcal{A}e^{ik_F S}\bar{u})/\hbar](\mathbf{r}) \sim -2i\hbar k_F \mathcal{A}(\mathbf{r}) e^{ik_F S(r;\hat{\mathbf{n}})/\hbar}(\nabla S)\cdot(\nabla \bar{u})^{1} \tag{2.5}$$

where $\mathcal{H}_0 + U(\mathbf{r}) = \frac{\hbar^2}{2m}(\nabla - \frac{ie\mathbf{A}}{c})^2 - \mu + \mathrm{U}(\mathbf{r})$ is the single particle hamiltonian. Thus the task of solving the full BdG eigenproblem (1.27) and (1.28) is reduced to the task of solving the classical Hamilton-Jacobi equation along with the (2x2) first order differential eigenproblem

$$\begin{pmatrix} -2i\hbar(k_F/m)\nabla S\cdot\nabla & \Delta_{eff}(x;\hat{\mathbf{n}}) \\ \Delta^*_{eff}(x;\hat{\mathbf{n}}) & 2i\hbar(k_F/m)\nabla S\cdot\nabla \end{pmatrix} \begin{pmatrix} \bar{u}_n(\mathbf{r}) \\ \bar{v}_n(\mathbf{r}) \end{pmatrix} = E_n \begin{pmatrix} \bar{u}_n(\mathbf{r}) \\ \bar{v}_n(\mathbf{r}) \end{pmatrix} \tag{2.6}$$

In fact, the eigenproblem is an *ordinary* rather than a *partial* differential equation. To see this, we recall the element of Hamilton-Jacobi theory in which one establishes that the solution S of the Hamilton-Jacobi equation (at least for classically allowed regions) is indeed the action computed along the classical trajectory $x_c(t)$ [15]. This in the simplest approximation is equivalent to a replacing $\hbar\nabla S\cdot\nabla$ with $\hat{\mathbf{n}}\cdot\nabla$ [2]. The semi-classical BdG equation then can be simply written as

$$\hat{H}_{Andreev} \begin{pmatrix} \bar{u}_n(\mathbf{r}) \\ \bar{v}_n(\mathbf{r}) \end{pmatrix} = E_n \begin{pmatrix} \bar{u}_n(\mathbf{r}) \\ \bar{v}_n(\mathbf{r}) \end{pmatrix} \tag{2.7}$$

with

$$\hat{H}_{Andreev} \equiv \begin{pmatrix} -2i(\mathbf{k}_F/m)\cdot\nabla & \Delta_{eff}(x;\hat{\mathbf{n}}) \\ \Delta^*_{eff}(x;\hat{\mathbf{n}}) & 2i(\mathbf{k}_F/m)\cdot\nabla \end{pmatrix}. \tag{2.8}$$

[1] Note that the potential $U_0(\mathbf{r})$ does not appear on the left-hand side of equation (2.5), since we assume S and $\mathcal{A}$ to be the solutions of Hamilton-Jacobi equations (equations (2.2) and (2.3))

[2] We should recall that the action along a classical trajectory can be written as $S_c = \mathbf{p}\cdot\mathbf{r}$, where $\mathbf{p}$ is the momentum along the direction of the trajectory, since we have assumed that the electrons are basically on the Fermi surface, $|\mathbf{p}| = \hbar k_F$

2.2 Analytical Solutions for the Quasi-Classical equation

We will simplify the quasi-classical approximation explained in the previous section by writing the Bogoliubov amplitudes in the form

$$\begin{pmatrix} u_n(\mathbf{r}) \\ v_n(\mathbf{r}) \end{pmatrix} = \exp(i\mathbf{k}_F \cdot \mathbf{r}) \begin{pmatrix} \bar{u}_n(\mathbf{r}) \\ \bar{v}_n(\mathbf{r}) \end{pmatrix} \tag{2.9}$$

and rewriting (2.7) as:

$$\begin{aligned} E\bar{u}_n &= -i\hbar\mathbf{v}_F \cdot \nabla\bar{u}_n(\mathbf{r}) + \Delta(\mathbf{r})\bar{v}_n(\mathbf{r}) \\ E\bar{v}_n &= i\hbar\mathbf{v}_F \cdot \nabla\bar{v}_n(\mathbf{r}) + \Delta(\mathbf{r})\bar{u}_n(\mathbf{r}) \end{aligned} \tag{2.10}$$

where $\mathbf{v}_F = \hbar\mathbf{k}_F/m$ is the velocity of an electron on the Fermi surface, we also simply write $\Delta_{eff}(x;\hat{\mathbf{n}})$ as $\Delta(\mathbf{r})$.

The quasi-classical approximation, i.e., neglecting $\hbar^2\nabla^2$ from the BdG equation, is equivalent to the fact that the pair-potential does not change appreciably over atomic distances. This also amounts to neglecting terms of order $(E^2 - \Delta^2)/E_F$ and $\hbar\nabla\Delta/k_F$ compared to E.

To be able to obtain self-consistent analytical solutions for the BdG in the quasi-classical regime, we restrict ourselves to the case of linear geometries (i.e. plane boundaries) so that the pair-potential in (2.10) depends on just one spatial coordinate, z. Assuming that $\bar{u}$ and $\bar{v}$ also depend only on z we can write [20]

$$\mathbf{v_F} \cdot \nabla \to v_F \cos(\theta) d/dz \qquad \cos(\theta) = \hat{\mathbf{v}}_F \cdot \hat{\mathbf{z}}. \tag{2.11}$$

We can decouple (2.10) by a simple transformation and investigate solutions for each equation separately. The strength of the quasi-classical approximation is in the fact that we can decouple the equations to a second-order *Schrodinger-like* equation for which analytical solutions can be found given a pair-potential.

Decoupling is achieved by introducing the complex combinations:

$$f_{1,n}(z,\cos\theta) \equiv \bar{u}_n(z,\cos\theta) + i\bar{v}_n(z,\cos\theta)$$
$$f_{2,n}(z,\cos\theta) \equiv \bar{u}_n(z,\cos\theta) - i\bar{v}_n(z,\cos\theta). \tag{2.12}$$

Rewriting (2.9) in terms of f_1 and f_2 we will have

$$E_n f_{1,n} = \hat{\Theta}_1 f_2 \equiv [-i\hbar v_F \cos\theta \frac{d}{dz} + i\Delta] f_{2,n}$$
$$E_n f_{2,n} = \hat{\Theta}_2 f_1 \equiv [-i\hbar v_F \cos\theta \frac{d}{dz} - i\Delta] f_{1,n} \tag{2.13}$$

where $\hat{\Theta}_1$ and $\hat{\Theta}_2$ are operators defined above.

Now, operating with Θ_2 on equation(2.12a) and with Θ_1 on equation (2.12b) yields two decoupled second-order equations. Using index l to distinguish $f_{1,n}$ and $f_{2,n}$ we can write our Schrödinger-like equations as

$$E_n^2 f_l = \{-[\hbar v_F \cos\theta]^2 \frac{d^2}{dz^2} + \Delta^2 - (-1)^l \hbar v_F \cos\theta \frac{d\Delta}{dz}\} f_{l,n} \tag{2.14}$$

Note that the eigenvalues are positive and also that the "potential" appearing in this Schrodinger equation contains both the pair-potential and its derivative. This appearance of $d\Delta/dz$ is a manifestation of the non-local behavior of superconductors, which is hidden in the BdG equation.

As will be seen later the special form of (2.12) leads us to a *Supersymmetric Quantum Mechanics(SUSY QM)* consideration of the quasi-classical BdG. We will devote a section particularly to this fact where, we will show that the reason we are able to do the following detailed calculation comes from the Supersymmetry of the quasi-classical BdG. [5]

Another important comment is that, we could do the same procedure to decouple the BdG itself, but instead of (2.13) we would end up with a fourth order equation:

$$\left[\left(-\frac{\hbar^2\nabla^2}{2m}+U(\mathbf{r})-\mu\right)^2+\Delta^2(\mathbf{r})\pm\frac{i\hbar^2}{2m}(\nabla^2\Delta)\right]f_{\pm,n}=E_n^2 f_{\pm,n} \qquad (2.15)$$

As one can see, the role of the quasi-classical approximation is to find analytical solutions since it is hard to find any for the BdG or the decoupled equation (2.14).

2.2.1 Ansatz Pair-Potentials

To be able to have self-consistent solutions, we will look for some *Ansatz* pair-potentials such that the resulting $\bar{u}_n$ and $\bar{v}_n$ satisfy the self-consistency relation $\Delta(\mathbf{r}) = g\sum_n u_n(\mathbf{r})v_n^*(\mathbf{r})(1-2f_n)$. To be able to do this, we need to include free parameters in our ansatz pair potential and fix them by demanding the self-consistency relations be satisfied. The satisfaction is not exact and in most cases we are actually only able to obtain a good self-consistent solution near T_c as will be seen later.

In the literature three Ansatz's have been considered and analytical solutions have been obtained (Δ_0 is the gap parameter in the bulk):

1) $\Delta(z) = \Delta_0 \tanh(\alpha z)$ [20].

2) $\Delta(z,T) = \Delta_0 + \Delta_1(T)e^{-z/\xi(T)}$ [18].

3) $\Delta(z) = \frac{\Delta_0}{1+e^{-\alpha z}}$ [14].

where α, ξ and Δ_1 are parameters to be determined.

In what follows, we will show in detail how the calculations work for Ansatz(1) near $T \sim T_c$. For (2) and (3) the self-consistency is only implicitly satisfied by variational methods to minimize the free energy.

2.2.2 Exact solutions

Introducing the new parameter X as

$$\Delta(z) = \Delta_0 X \equiv \Delta_0 \tanh(\alpha z) \tag{2.16}$$

and convenient dimensionless parameters

$$\overline{E} = E/\Delta_0(T)$$
$$\nu^{-1} = \alpha \hbar v_F \cos(\theta)/\Delta_0(T) \tag{2.17}$$

and rewriting equation (2.13) in terms of X using the relation $d/dz = \alpha(1 - X^2)(d/dX)$ we end up with

$$(1 - X^2)\frac{d^2 f_l}{dX^2} - 2X\frac{df_l}{dX} + \{\nu[\nu - (-1)^l] - \frac{\mu^2}{(1 - X^2)}\} f_l = 0 \tag{2.18}$$

where $l = 1, 2$ and

$$\mu = \nu(1 - \bar{E}^2)^{1/2}. \tag{2.19}$$

For $E > \Delta_0$, the parameter μ is pure imaginary, while for $E < \Delta_0$, μ is real. Now it is easy to see that the solutions of (2.18) are Legendre functions of the first and second kinds:

$$f_{1,n}(z, cos\theta) = P_\nu^{\pm\mu}(z) \quad or \quad Q_\nu^{\pm\mu}(z)$$
$$f_{2,n}(z, cos\theta) = P_{-\nu}^{\pm\mu}(z) \quad or \quad Q_{-\nu}^{\pm\mu}(z) \tag{2.20}$$

where μ and ν are functions of $\cos\theta$.

If μ is not a real integer, P_ν^μ and $P_{-\nu}^\mu$ are two independent solutions and then we need not introduce Legendre functions of the second kind, explicitly. Only when E is less than Δ_0 can μ be a real integer. But then Q_ν^μ does not decay far from the boundary as it should, and therefore it is not acceptable as a solution.

Before dealing with the self-consistency criterion, we should normalize the solutions obtained so far, For scattering states we just look at the behavior of the solutions in the limit $z \to \infty$ where we expect Δ to be constant. Expressing the Legendre functions in terms of the Hypergeometric function, we have

$$P_\nu^{i|\mu|}(X) = \left(\frac{1-X}{1+X}\right)^{i|\mu|/2} F(-\nu, 1+\nu, 1-\mu; \frac{1}{2} - \frac{1}{2}X)/\Gamma(1-i|\mu|)$$
$$= e^{iqz} F/\Gamma(1-i|\mu|) \qquad (2.21)$$

where $\Gamma(x+1) = x!$ and

$$q \equiv (E^2 - \Delta_0^2)^{1/2}/(\hbar v_F \cos\theta). \qquad (2.22)$$

As $z \to \infty$ (i.e. as $\frac{1}{2} - \frac{1}{2}X \to 0$), $F \to 1$, so we retain the free wave-functions. Demanding that they coincide with the BCS solutions give rise to

$$\begin{pmatrix} f_1 \\ f_2 \end{pmatrix}_{bulk} = \begin{pmatrix} u_0 + iv_0 \\ u_0 - iv_0 \end{pmatrix} e^{qz} = \begin{pmatrix} e^{i\phi} \\ e^{-i\phi} \end{pmatrix} \qquad (2.23)$$

where u_0 and v_0 are the BCS parameters

$$u_0^2 = 1 - v_0^2 = \frac{1}{2}(1 + \varepsilon/E) \qquad (2.24)$$

and

$$\phi = \tan^{-1}(v_0/u_0). \qquad (2.25)$$

When ε changes sign, the solution is obtained by the transformation

$$\varepsilon \to -\varepsilon \quad \Rightarrow u_0 \longleftrightarrow v_0 \Rightarrow e^{i\phi} \to ie^{-i\phi}, e^{-i\phi} \to -ie^{i\phi}. \qquad (2.26)$$

Noticing that $u = \exp[ik_F(z\cos(\theta) + \rho\sin(\theta)]\bar{u}$ where ρ is the cylindrical polar coordinate perpendicular to z, it is obvious that for a given energy E and a wave

vector parallel to the boundary surface $k = k_F \sin(\theta)$ there are four solutions corresponding to the four combinations of the value

$$a = sgn(\cos\theta), \quad b = sgn(\varepsilon). \tag{2.27}$$

Inserting the phase obtained in equation (2.26) and considering the four possible solutions obtained so far through the introduction of a and b the solutions can be written as

$$\begin{pmatrix} f_1 \\ f_2 \end{pmatrix} = \Gamma(1 - iab|\mu|) \begin{pmatrix} e^{ib\phi} P_{a\nu}^{iab|\mu|}(X) \\ e^{-ib\phi} P_{-a\nu}^{iab|\mu|}(X) \end{pmatrix} \exp(iak_F|\cos\theta|z) \tag{2.28}$$

where $b = +1$ (i.e., $\varepsilon > 0$) corresponds to the quasi-electron excitation and $b = -1$ (i.e., $\varepsilon < 0$) to a quasi-hole. The condition $ab = +1(-1)$ corresponds to the forward (backward) propagation. We have then fixed the relative phase as well as the total normalization of the scattering states.

We also can go through the normalization of bound-states, but as it turns out that their contribution in self-consistency relations is very small, we skip this and focus on the last step, which is finding the Δ_0 so that we get the approximate self-consistent solutions.

2.2.3 Requirement of Self-consistency

In the older works [17] self-consistency is shown to be satisfied near T_c for a special value of α using only the leading terms of the self-consistency relation. Following the same approach we were able to show that the calculation with the already determined value of α, also taking into account almost all of the effective terms in equation (1.39) using a Mathematica code, can be generalized to lower temperature.

In the following we just briefly review the analytical calculations that contain some inevitable approximations

Assuming the boundary conditions to be (first index for $\Psi$is 'a' and second is 'b'),

$$\Psi = A\Psi_{1,1} + B\Psi_{1,-1} + C\Psi_{-1,1} = 0. \tag{2.29}$$

with Ψ denoting the spinor wave-function. The coefficients A, B and C can be shown to be [20]:

$$\begin{aligned} A &= e^{-2i\phi} P_{\nu}^{i|\mu|}(0)^2 + e^{2i\phi} P_{-\nu}^{i|\mu|}(0) \\ B &= |P_{-\nu}^{i|\mu|}(0)|^2 - P_{\nu}^{i|\mu|}(0)^2 \\ C &= -2Re(e^{2i\phi} P_{-\nu}^{i|\mu|}(0) P_{\nu}^{i|\mu|}(0)). \end{aligned} \tag{2.30}$$

we write the uv^* term that enters the self-consistency relation as:

$$uv^* = \frac{1}{4}(|f_1|^2 - |f_2|^2) + \frac{1}{2} Im(f_1 f_2^*). \tag{2.31}$$

It is important to note that the imaginary part of (2.30) vanishes due to the symmetry between electrons and holes which can be easily verified using (2.12)

For scattering states with boundary condition (2.30) this term is written as

$$\begin{aligned} (uv^*)_{scat} &= 2Im(e^{2i\phi} P_{-\nu}^{i|\mu|}(X) P_{\nu}^{i|\mu|}(X) |\Gamma(1+\mu)| + \\ (B/A^*) P_{-\nu}^{i|\mu|}(X) P_{\nu}^{i|\mu|}(X) [\Gamma(1-\mu)]^2 + \ldots &= 2\Xi_1 + 2\Xi_2 + O.T. \end{aligned} \tag{2.32}$$

where O.T. designates spatially oscillating terms. To maintain self-consistency with the quasi-classical approximation, which basically assumes no oscillation of Δ on λ_F scale, we drop these rapidly oscillating terms.

It is now, convenient to write the Legendre function appearing in (2.20) in terms of the Hypergeometric function, using the expansion for Hypergeometric functions

$$F(a,b,c;\zeta) = \sum_{n=0}^{\infty} \frac{a_n b_n}{c_n} \frac{\zeta^n}{n!}. \tag{2.33}$$

For our case, $\zeta = \frac{1}{2} - \frac{1}{2}X, a = -\nu, b = +\nu$, $c = 1 - \mu$. This series is also an expansion in $\nu/|\mu| = \Delta/\varepsilon \propto \Delta_0$ so we can approximate the sum with just the first few terms in the limit of $T \to T_c(\Delta_0 \to 0)$.

Inserting the expansion in (2.31) and after some straightforward calculations we finally end up with

$$\Pi \equiv e^{2i\phi} P_{-\nu}^{i|\mu|}(X) P_{\nu}^{i|\mu|}(X) |\Gamma(1+\mu)| = 1 - 2(\zeta/\varepsilon^2) + i[2(\zeta/\varepsilon) + 2(\zeta/\varepsilon|\mu|^2) - 6(\zeta^2/\varepsilon|\mu|^2) - 4(\zeta^3/\varepsilon^3) + 4(\zeta^3\varepsilon|\mu|^2)] + O(|\mu|^{-4}). \tag{2.34}$$

Multiplying by the factor $\exp(i\phi)\tanh(\frac{1}{2}\beta E)$ and taking the imaginary part, we find for Ξ_1

$$\Xi_1 \tanh(\frac{1}{2}\beta E) = [\frac{\Delta_0}{E}(1-2\zeta) - \frac{\Delta_0}{E}\varepsilon^{-2}(1-\varepsilon^2/|\mu|^2)(2\zeta + 6\zeta^2 + 4\zeta^3)] \times \tanh(\frac{1}{2}\beta E) + \ldots = [X(\delta_0/E) - \frac{1}{2}(\Delta^3/\varepsilon^2 E)X(1-X^2)(1-\nu^{-1})] \times \tanh(\frac{1}{2}\beta E) \tag{2.35}$$

remembering that $1 - 2\zeta = X$.

If we keep only the first term in equation(2.35), the self-consistency condition reduces to that of BCS, and fails to determine α. To find α, we demand that the contribution from the second term shall vanish. Integrating over angles we require

$$\int_0^1 (1-\nu^{-2}) d\cos\theta = \int_0^1 [1 - (\hbar v_F \alpha/\Delta_0)^2 \cos^2(\theta)] d\cos\theta = 1 - \tfrac{1}{3}(\hbar v_F \alpha/\Delta_0)^2 = 0. \tag{2.36}$$

which means

$$\alpha = \sqrt{3}\Delta_0(T)/\hbar v_F \tag{2.37}$$

This is in agreement with the Ginzburg-Landau value, $\alpha = 1/\sqrt{2}\xi(T)$ as we should expect, since we know from Gor'kov's original work [10] that the Landau-Ginzburg theory is asymptotically correct as we approach T_c.

2.3 Quasi-Classical equation and Supersymmetric Quantum Mechanics

The analytical solutions obtained in terms of Legendre polynomials in the previous section and the variety of other self-consistent solutions all in terms of well-known orthogonal polynomials are not accidental. The existence of such solutions with the Ansatz pair potentials $\Delta_0 \tanh(\alpha x)$, $\Delta_0 + \Delta_1 \exp(-\alpha x)$ and $\Delta_0/[1 + \exp(-\alpha x)]$ is a result of the *Supersymmetry* of the quasi-classical BdG equation.

In our problem, supersymmetry tells us why particular ansatz pair-potentials will work while others fail to give analytical solutions, and can be seen as a generalization of mathematical tricks that Bar-Sagi and Kuper performed [17] to obtain the Legendre equation.

We begin with the quasi-classical equation:

$$\begin{pmatrix} \mathcal{H}_0(x;\hat{\mathbf{n}}) & \Delta_{eff}(x;\hat{\mathbf{n}}) \\ \Delta^*_{eff}(x;\hat{\mathbf{n}}) & -\mathcal{H}_0(x;\hat{\mathbf{n}})^* \end{pmatrix} \varphi_n(x;\hat{\mathbf{n}}) = E_n \varphi_n(x;\hat{\mathbf{n}}) \tag{2.38}$$

where

$$\varphi_n(x;\hat{\mathbf{n}}) = \begin{pmatrix} \bar{u}_n(\mathbf{r}) \\ \bar{v}_n(\mathbf{r}) \end{pmatrix} \tag{2.39}$$

and

$$\mathcal{H}_0 = v_F \hat{\mathbf{n}} \cdot (\mathbf{p} - \frac{e}{c}\mathbf{A}). \tag{2.40}$$

The idea of writing the quasi-classical BdG in the form of a *Schrodinger-like* equation is as a result of the fact that the square of the quasi-classical Hamiltonian, $\hat{\Omega}$, (for simplicity we assume zero magnetic field) [5]

$$\hat{\Omega} = \begin{pmatrix} \mathcal{H}^2 + \Delta^2 & [\mathcal{H}, \Delta] \\ -[\mathcal{H}, \Delta] & \mathcal{H}^2 + \Delta^2 \end{pmatrix} = \begin{pmatrix} -\hbar^2 v_F^2 \partial_x^2 + \Delta^2 & -i\hbar v_F(\partial_x \Delta) \\ i\hbar v_F(\partial_x \Delta) & -\hbar^2 v_F^2 \partial_x^2 + \Delta^2 \end{pmatrix} \tag{2.41}$$

can be diagonalized using the simple unitary transformation

$$\mathcal{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}, \quad \mathcal{U}^\dagger = \mathcal{U}^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \tag{2.42}$$

i.e.,

$$\hat{\Omega}' = \equiv \mathcal{U}^\dagger \hat{\Omega} \mathcal{U} = \begin{pmatrix} H_+ & 0 \\ 0 & H_- \end{pmatrix} \tag{2.43}$$

where

$$H_\pm = -\hbar^2 v_F^2 \partial_x^2 + \Delta^2 \pm \hbar v_F(\partial_x \Delta). \tag{2.44}$$

In the context of SUSY Quantum Mechanics, Δ is called the *Superpotential* and directly enters the definition of the ladder operators Q and $Q^\dagger$ which are defined as:

$$Q \equiv -\hbar v_F \partial_x + \Delta, \qquad Q^\dagger = \hbar v_F \partial_x + \Delta, \tag{2.45}$$

as

$$H_+ = Q^\dagger Q, \quad H_- = Q Q^\dagger. \tag{2.46}$$

The ladder operators, Q and $Q^\dagger$, switch the eigenfunctions of H_+ and H_-, say $\varphi_\pm$ through:

$$\varphi_{-,n} = \frac{1}{|E_n|} Q\varphi_{+,n}, \quad \varphi_{+,n} = \frac{1}{|E_n|} Q^\dagger \varphi_{-,n}. \tag{2.47}$$

The most important feature of SUSY Quantum mechanics is that we can analytically calculate both the spectrum and the eigenfunctions of the partner Hamiltonians $H_\pm$ by means of simple algebraic manipulation, provided that the "potential" $U_\pm(x) = \Delta^2 \pm \hbar v_F(\partial_x \Delta)$ which enters in our Schrodinger-like equation is *shape invariant*, i.e., when:

$$U_+(x; a_0) = U_-(x; a_1) + R(a_1) \tag{2.48}$$

where a_1 is a new set of parameters uniquely determined from the old ones a_0 and the residual term $R(a_1)$ is independent of x.

We can now easily see that all three proposed Ansatz pair-potentials satisfy the above condition. This is clear if we write them in the following forms:

$$\begin{aligned} \Delta(x; a_0) &= a_0 \tanh(\alpha x) \\ \Delta(x; a_0) &= 1 + a_0 \exp(-\alpha x) \\ \Delta(x; a_0) &= \frac{a_0}{1 + \exp(-\alpha x)} \end{aligned} \tag{2.49}$$

All the analytical solutions obtainable through SUSY Quantum Mechanics can be summarized in a table [42] which gives the eigenfunctions and energy spectrum for each proposed superpotential. It seems that the reason for only having three known self-consistent pair-potentials is more due to the practical technicalities than to a physical argument.

Chapter 3

Hubbard Model and discretized version of the Bogoliubov-de Gennes equation

3.1 Introduction

In the following section, we will show how the same procedure that led us to generalize the Hartree-Fock method in the normal metal to the superconducting case can be done for the strong-coupling regime for which Hamiltonians based on the tight-binding approximation, like the Hubbard model, are suitable. Though our derivation of the discrete Bogoliubov-de Gennes equation will be for a quite general form of the Hubbard model, the remaining sections will be devoted to numerical calculations to obtain the self-consistent solutions in a 1D s-wave superconductor within the nearest-neighbor tight-binding approximation. Different situations such as the BCS case (i.e., periodic boundary conditions (PBC)), finite size (or open boundary conditions (OBC)) and the effect of a single non-magnetic impurity will be investigated.

In certain regimes some interesting self-consistent solutions for the gap function near the boundaries will be presented and the results will be compared to that with periodic boundary conditions and with an on-site impurity (instead of

a boundary). It will be seen that the results from the two are similar but not quite the same thing.

The Local Density of States (LDOS) is almost the only quantity that can be measured directly using scanning tunneling microscopy(STM) so in this regard we examined LDOS in different situations, specially the cross-over from surface density of states to that in the bulk (representing the BCS density of states) we obtained the qualitative agreement with recent STM experiments and a non-magnetic impurity on the surface [7].

3.2 Theoretical considerations:

Although our calculations will be based on a simple s-wave tight-binding model, in this section I will present a fairly general derivation for the extended Hubbard model taking into account of off-site interactions as well.

Let's begin with extended Hubbard Hamiltonian written in the following form:

$$\hat{H}_{Hubbard} = -\sum_{ij,\sigma} t_{ij}(c^{\dagger}_{i\sigma}c_{i\sigma} + h.c.) - \sum_{i\sigma}(\mu + \epsilon_i)c^{\dagger}_{i\sigma}c_{i\sigma} + \sum_{i} U_i n_{i\uparrow}n_{i\downarrow} + \sum_{ij\sigma} V^{\sigma}_{ij} n_{i\sigma}n_{j\sigma} \tag{3.1}$$

where $n_{i\sigma} \equiv c^{\dagger}_{i\sigma}c_{i\sigma}$ and the creation and annihilation operators, $c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$ respectively, create and annihilate electrons with spin σ at the lattice point i. t_{ij} is the amplitude for hopping from site i to j, and vice versa. U_i is the interaction energy of two electrons with opposite spins at the site i and is responsible for pairing in the Hubbard model. For the sake of generality we have included position dependent site energy ϵ_i (which is non-zero for systems containing impurities) and also the general density-density interaction term V_{ij}.

There are different ways to introduce inhomogeneity effects, it can come from the fact that hopping probability is not constant (in the simplest case, for finite

sizes, it is some constant t_1 inside the system and t_2 outside). The hopping from inside to outside, $t_{1\to 2}$ (and vise versa) can be different from both t_1 and t_2. The pairing strength U can be site dependent [43] [33] and finally ϵ_i is the position dependent part of chemical potential in our model indicates whether there is any impurity on site i or not. It can also play the role of boundary potential by assuming large ϵ_i near the boundaries.

The procedure of obtaining BdG is exactly the same as in chapter 1. We introduce the local expectation values

$$a_i \equiv < c_{i\downarrow} c_{i\uparrow} > \tag{3.2}$$

$$b_{ij} \equiv < c_{i\downarrow} c_{j\uparrow} > \tag{3.3}$$

and the local order parameters

$$\Delta_{ii} \equiv -U_i a_i \tag{3.4}$$

$$\Delta_{ij} \equiv -V_{ij} \frac{b_{ij} + b_{ji}}{2} \tag{3.5}$$

Performing a mean field decoupling of the interactions in equation (3.1)and a Bogoliubov transformation to quasi-particle operators we obtain the BdG equation in the following form

$$\sum_j \mathbf{H}_{ij}^{BdG} \begin{pmatrix} u_{n,i} \\ v_{n,i} \end{pmatrix} = E_n \begin{pmatrix} u_{n,i} \\ v_{n,i} \end{pmatrix} \tag{3.6}$$

where

$$\mathbf{H}_{ij}^{BdG} \equiv \begin{pmatrix} H_{ij} & \Delta_{ij} \\ \Delta_{ij}^* & -H_{ij}^* \end{pmatrix} \tag{3.7}$$

with H_{ij} defined as,

$$H_{ij} \equiv -t_{ij} - (\epsilon_i + \mu)\delta_{ij} \tag{3.8}$$

The only difference with the usual case is that the order parameter Δ , here, has off-diagonal matrix elements in addition to diagonal ones. The self-consistency conditions are

$$\Delta_{ii} = -U_i \sum_n u_{n,i} v^*_{n,i} (1 - 2f_n) \tag{3.9}$$

$$\Delta_{ij} = \frac{V_{ij}}{2} \sum_n (u_{n,i} v^*_{n,j} + u_{n,j} v^*_{n,i})(1 - 2f_n) \tag{3.10}$$

with f_n the fermi function for energy E_n as usual.

It is worth noticing that we could begin from Hamiltonian (1.5) and its effective counterpart (where off-diagonal elements for Δ is assumed and the quadratic term in Δ is ignored for simplicity).

$$\hat{H}_{eff} = \int d^3r [\psi^\dagger_\alpha(\mathbf{r}) \mathcal{H}_0 \psi_\alpha(\mathbf{r}) + \psi^\dagger_\alpha(\mathbf{r}) U(\mathbf{r}) \psi_\alpha(\mathbf{r})] + [\int \int d^3r' d^3r \\ \Delta(\mathbf{r}', \mathbf{r}) \psi^\dagger_\uparrow(\mathbf{r}) \psi^\dagger_\downarrow(\mathbf{r}') + \Delta^*(\mathbf{r}) \psi_\downarrow(\mathbf{r}) \psi_\uparrow(\mathbf{r}')] \tag{3.11}$$

and obtain the BdG as formulated above following the usual tight-binding techniques.

This is obtained by introducing *wannier functions*, $w_i(\mathbf{r})$, and transforming field operators as

$$\psi_\sigma(\mathbf{r}) = \sum_i w_i(\mathbf{r}) c_{i\sigma} \tag{3.12}$$

$$\psi^\dagger_\sigma(\mathbf{r}) = \sum_i w^*_i(\mathbf{r}) c^\dagger_{i\sigma} \tag{3.13}$$

Requiring the following properties for wannier functions (that also guarantee their uniquness).

- $w_i(\mathbf{r})$ are orthonormal.

- $w_i(\mathbf{r})$ is localized around site number i.
- every $w_i(\mathbf{r})$ is a linear combination of Bloch wave-functions.

we can relate parameters in equation (3.1) and equation (3.11), as

$$t_{ij} = \int d^3r w_i^*(\mathbf{r}) \mathcal{H}_0 w_j(\mathbf{r}) \tag{3.14}$$

$$\Delta_{ij} = \int d^3r d^3r' w_i^*(\mathbf{r}') \Delta(\mathbf{r}, \mathbf{r}') w_j(\mathbf{r}) \tag{3.15}$$

An important point here is since wannier functions are localized around lattice points, we can use Δ_i instead of $\Delta(\mathbf{r})$ to represent the gap value at lattice point i.

3.2.1 Simplified model in the presence of boundaries

To simplify the model to make the computations possible, we assume that since $w_i(\mathbf{r})$ and $w_j(\mathbf{r})$ do not overlap so much unless i and j are neighboring sites (this come from the fact that wannier functions are localized) the integral in equation(3.14a) is non-zero just for nearest neighbors.

Also to be able to deal with finite size systems (i.e., open boundary conditions) we can imagine a high potential barrier form for $U^{(0)}(\mathbf{r})$ from the beginning, then one can see that the terms $t_{1,0}$ and $t_{N,N+1}$, where by 0 and $N+1$ we mean first sites that lie outside the system, will be affected dominantly by this potential (if we assume a potential that abruptly changes near the boundary from a high value outside the superconductor to zero inside, and assuming that the variations are step-function like, then from equation (3.14) we can see that $t_{1,0} = t_{N,N+1} = 0$.

And finally for the sake of simplicity again we put Hartree potential equal to it's mean field value $n_e|U|/2$ where n_e is the average electron density per site, though this seems an oversimplification, from [4] we know that the superconducting behavior wouldn't be changed so much by this assumption.

3.3 How the BdG code works:

The program (written in C) uses some fixed parameters such as the pairing strength $|U|$, electron density n_e, and temperature T and also some initial guesses for the chemical potential μ and pair-potential Δ_i . Since the rate of convergence of the program depends on these initial guesses, they were changed from situation to situation to speed up the convergence of the program.

The program works according to the following steps:

(I). First we write the BdG equation with t_{ij} equal to a constant t for nearest-neighbor hopping only. H_{BdG} can be written as a $2N \times 2N$ matrix:

$$\left(\begin{array}{cccc|cccc} -\tilde{\mu} & -t & 0 & \cdots & \Delta_1 & & & \\ -t & -\tilde{\mu} & -t & 0 & & \Delta_2 & \cdots & \\ 0 & -t & -\tilde{\mu} & -t & & & \Delta_3 & \\ c & \cdots & -t & -\tilde{\mu} & \cdots & & & \Delta_4 \\ \hline \Delta_1^* & & & & \tilde{\mu} & t & \cdots & -c \\ & \Delta_2^* & & \cdots & t & \tilde{\mu} & t & 0 \\ & & \Delta_3^* & & 0 & t & \tilde{\mu} & t \\ & \cdots & & \Delta_4^* & -c & \cdots & t & \tilde{\mu} \end{array}\right) \tag{3.16}$$

where $\tilde{\mu} \equiv \mu - n_e U/2$. c is zero for open boundary conditions and $-t$ for periodic ones (since, $t_{1,N} = t_{n,1} = -t$ for PBC).

In the first step, the program diagonalizes H_{BdG}, calling the function "jacobi.c" that uses the Jacobi method to diagonalize an arbitrary matrix by applying a few number of unitary transforms, the number depends on how far from a diagonal the matrix is. The standard "jacobi.c" also provides us with the number of rotations needed for diagonalizing the matrix too. It writes the eigenvectors $(u_{n,i}, v_{n,i})$ in a $2N \times 2N$ matrix v_{ij} and eigenvalues E_n in a $2N$-dimensional vector l_i. Also, it calls "eigsrt.c" to sort out the

eigenvalues and their corresponding eigenvectors which is crucial when we have degeneracies (which is the case almost all the times).

(II). In this step we calculate the corresponding potentials Δ_i and U_i according to the self-consistency relations. It is important to emphasize that since we are interested in the different behavior of different physical quantities as a function of electron density n_e rather than chemical potential μ, there is one more criteria to be satisfied with the BdG to obtain self-consistency, which is the number equation. We will explain this point later on in more detail.

On applying the self-consistent relations we note a symmetry of the BdG equations: Under transformation,

$$\begin{aligned} (u_{n,i}, v_{n,i}) &\mapsto i\hat{\tau}_2(u^*_{n,i}, v^*_{n,i}) \\ E_n &\mapsto -E_n \end{aligned} \tag{3.17}$$

the BdG equations are invariant (τ_2 is the Pauli matrix). This symmetry requires us to take account of positive energy eigenvalues only in the BdG equation, since the equation (3.17) indicates that both wave-functions with negative eigenvalue E_n can be expressed in terms of ones with positive energy.

(III). To check whether we have achieved self-consistency, we check the difference between $\Delta_i^{(N)}$ and $\Delta_i^{(N-1)}$ where N indicates the Nth iteration (conveniently, instead of doing it for all the i's the program only does it for i in the middle of the system) then, we compare the relative difference with a fixed tolerance δ (we used 0.0001). Once the condition

$$\frac{\Delta^{(N)} - \Delta^{(N-1)}}{\Delta^{(N-1)}} \leq \delta$$

is satisfied, we stop the iteration and have obtained the self-consistent solutions given μ_0 as the initial chemical potential.

(IV). We need to solve the number equation for μ, given n_e:

$$n_e = f(\mu; u_{n,i}, v_{n,i}, E_n).$$

This can be done by the Newton-Raphson method that I briefly explain in the following:

1. Having a guessed value μ_0 the code calculates $f(\mu_0)$ and $f(\mu_0 + \delta\mu)$ where $\delta\mu$ is a very small constant.
2. A line is drawn that passes from the points $(\mu_0, f(\mu_0))$ to $(\mu_0 + \delta\mu, f(\mu_0 + \delta\mu))$ and the value of μ_1 found to give $f(\mu_1) = 0$.
3. The same steps are repeated until μ_1 reaches a fixed point.

   If someone tries to do the above steps with non-self consistent solutions there is no guarantee for the convergence of this procedure, or it may be very slow. Thus, every time we calculate $f(\mu; u_{n,i}, v_{n,i}, \varepsilon_n)$ we should call the previous steps (I)-(IV) to solve the BdG equation self-consistently.

3.4 Checking the code with known BCS results

Before we proceed with the physically relevant regimes, we should make sure that the solutions are correct, so I used a FORTRAN program, "bcs1d.f", that solves the non-linear BCS equations given the system size, electron density and pairing strength, to which I could compare my results obtained from solving BdG

with PBC with the same parameters used. The agreement was complete up to four decimal digits (note that all the energies and temperatures are measured in the units of hopping probability, t, i.e. $E, T \to E/t, T/t$) in all the different situations. This is a good test for the program since the behavior is already known in the BCS regime, and also remembering that BCS equations are basically obtained in a totally different way and also BCS gap equation is quite different with what we have in BdG.

The "bcs1d.f" program basically solves BCS equations, i.e:

$$1 = \frac{|U|}{2N} \sum_k \frac{1}{E_k} [1 - 2f(E_k)]$$

with

$$E_k = \sqrt{(\varepsilon_k^{(0)} - \mu - |U| n_e/2)^2 + \Delta_{BCS}^2}$$

and $\varepsilon_k^{(0)} = -2t \cos k$, where the sums are carried out over the first Brillouin zone $(-\pi < k \leq \pi)$. The code uses a finite lattice for simplicity, large enough for the gap to converge to its bulk limit. The auxiliary equation (the same as BdG) to determine the electron number density is also required

$$n_e = 1 - \frac{1}{N} \sum_k \frac{\varepsilon_k - \mu - |U| n_e/2}{E_k}$$

For a given U and n_e these equations are iterated to convergence to determine μ and Δ_{BCS}.

To test the program, first $\Delta_{Bulk}(i.e., \Delta(N/2))$ and first excitation energy ε_1 (let's call it E_{min}) are plotted versus n_e and the whole graph was done for afew different temperatures ranging from zero to near T_c. The result was an exact agreement between the two as can be seen from FIGs (1)-(3).

To get every point in Figures(3.1)-(3.3) from the BdG, we have to iterate the equations to self-consistency, that is much more time consuming than solving

BCS equations. Thus the resolution of the BdG curves is lower.

In all plots the pairing strength is kept constant to $2t$ (reminding that t is the hopping amplitude and all the energies are measured in units of t).

A very good sign is the so-called "even-odd effect" for E_{min} that can be seen exactly in the BdG results as well as the BCS ones. In the next section we will discuss about this in more detail and show the result obtained for OBC too.

Finally, different temperatures were done just as a double check of the agreement between BCS and BdG and although not much qualitatively new physical information obtained, we obtain results similar to what we had at zero temperature.

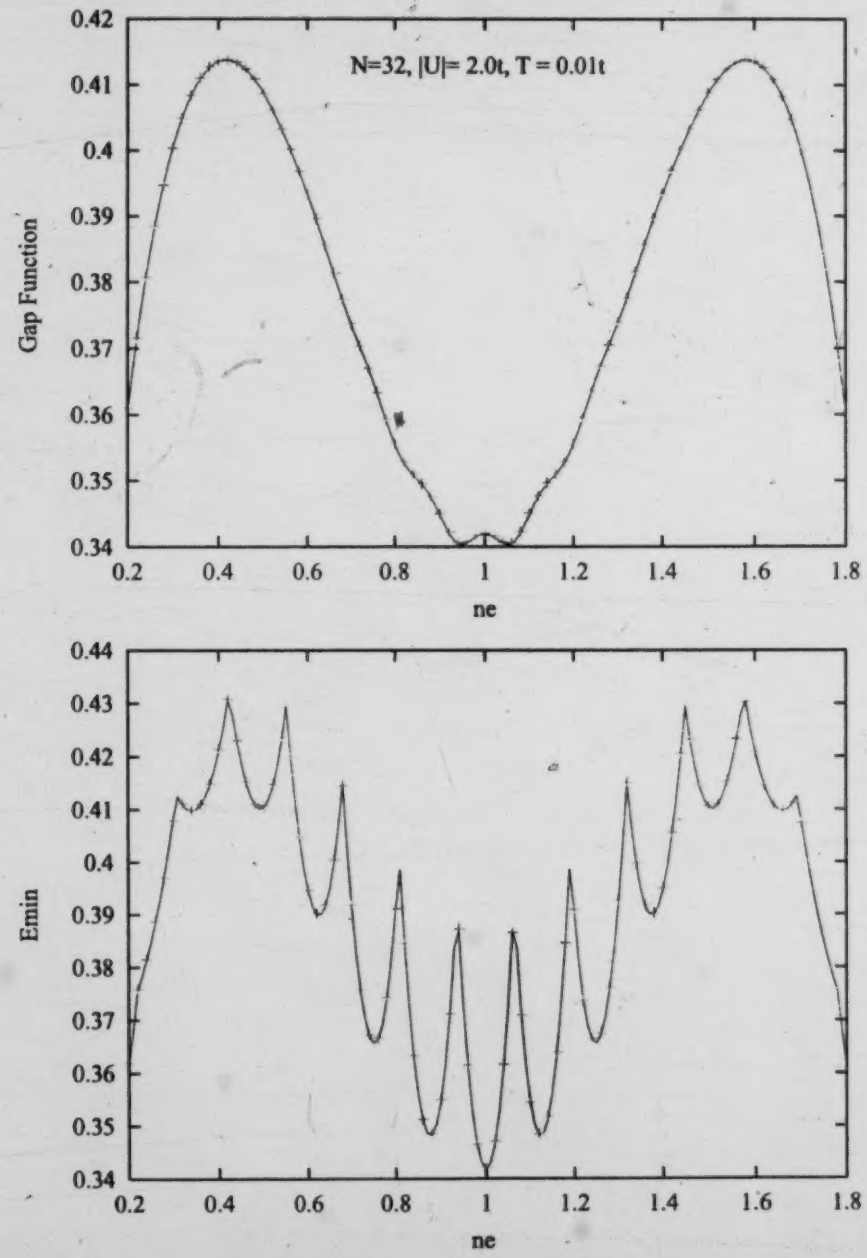

Figure 3.1: BCS (solid lines) and BdG results with periodic boundary conditions (plus signs). (up) Gap function vs. electron density, $n_e = N_e/N$ (where N_e is the total number of electrons and N is the number of sites) compared together, showing complete agreement.(down) The same but E_{min} (first excitation energy) is plotted vs. electron density (down). The temperature, T, is zero (actually $0.01t$), $N = 32$ and pairing strength, $|U|$, is $2t$.

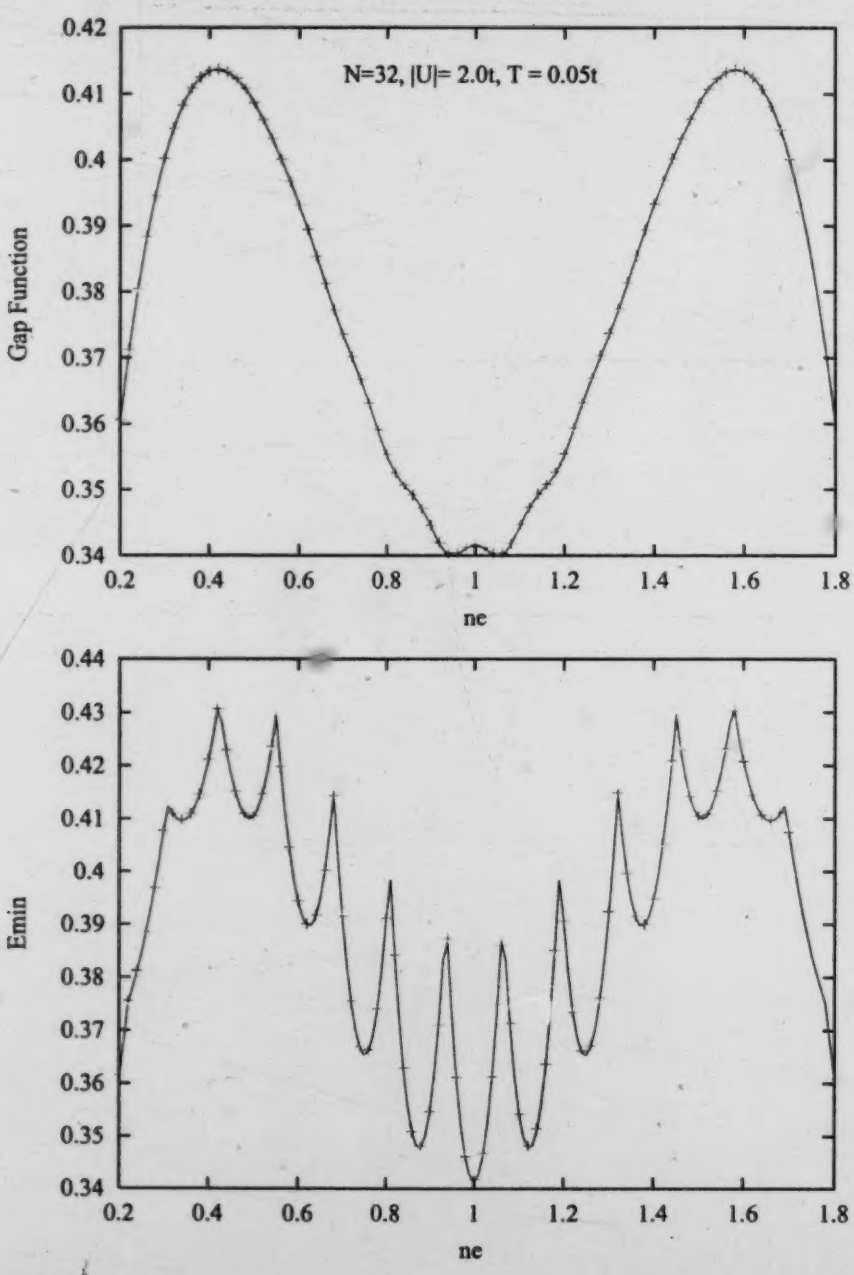

Figure 3.2: The same as FIG 3.1 with temperature T=0.1t (the transition temperature is 0.2t)

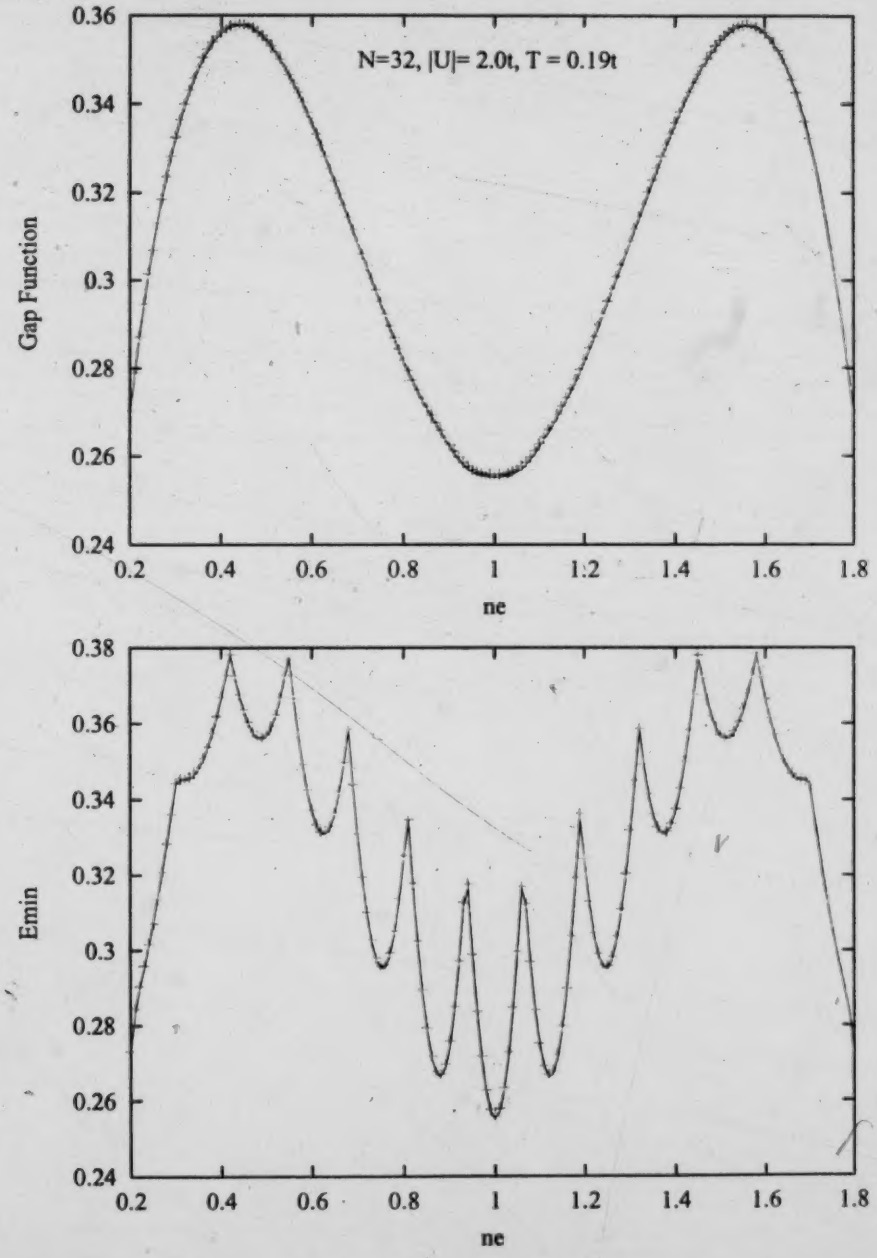

Figure 3.3: The same as FIG 3.1 with temperature T=0.15t (the transition temperature is 0.2t)

3.5 Open boundary conditions; deviation from BCS

In this section we follow what was presented in the previous section, but this time we will compare the results from BCS (or equivalently, BdG with periodic boundary conditions) with BdG with open boundary conditions. As well, the system with PBC but with a single non-magnetic impurity is considered. The transition to normal metal and the validity of the BCS and BdG equations near the critical point is investigated too.

The idea behind considering the impurity is two-fold. First we want to investigate by how far we can approximate an OBC system with a system with an impurity to account for the boundaries of the system, i.e., instead of the Hamiltonian

$$H = -\sum_{i}^{N}\sum_{\sigma} t(c^{\dagger}_{i+1\sigma}c_{i\sigma} + h.c.) - \sum_{i\sigma}\mu c^{\dagger}_{i\sigma}c_{i\sigma} - |U|\sum_{i} n_{\uparrow i}n_{\downarrow i} \tag{3.18}$$

with the open boundaries, we use the following Hamiltonian with a single impurity and with periodic boundary conditions

$$H = -\sum_{i}^{N}\sum_{\sigma} t(c^{\dagger}_{i+1\sigma}c_{i\sigma} + h.c.) - \sum_{i\sigma}(\mu + V_{impurity}\delta_{i,N})c^{\dagger}_{i\sigma}c_{i\sigma} - |U|\sum_{i} n_{\uparrow i}n_{\downarrow i} + (\sum_{\sigma} tc^{\dagger}_{N\sigma}c_{1\sigma} + h.c.) \tag{3.19}$$

where $-V_{impurity}$ is the impurity potential and $\delta_{i,N}$ indicates that the impurity is at site N . The particular choice of N is to help compare the results from OBC and PBC with an impurity. Note that because of the form of Hamiltonian introduced, to be able to compare the OBC case with PBC+impurity we should use systems with $N+1$ sites for the latter (one site for the single impurity)

Since there is no next-nearest-neighbor hopping assumed, if the hopping amplitude from a site next to the impurity is small compared with the impurity potential (i.e., $t \ll V_{impurity}$) then we expect good agreement between both cases.

The other reason to investigate the properties of the system near an impurity is the tunneling experiments that determine the conductivity (and so density of states) of the system at the surface of the superconductor. We will devote a separate subsection where we present our results obtained for the LDOS of the systems.

In Figures(3.4), (3.5), (3.6) and (3.7), it can be seen that there is a striking feature [27] , namely the difference between E_{min} for $N_e = 4m$ (N_e is the total number of electrons and m is an integer) and $N_e = 4m + 2$. The results for $N_e = 4m + 2$ are much larger than those for $N_e = 4m$. These oscillations have been called *super-even effect*: the system is more stable with $4m + 2$ electrons than with $4m$. This effect is more pronounced when the coupling is weak, and it stems from the quantized and doubly degenerate energy levels $\varepsilon_k + \varepsilon_{-k}$ (for BCS) of the unperturbed system. As can be shown when the coupling is weak, the occupation probabilities of the unperturbed states can be approximated by those for zero coupling. We can thus understand the effect as follows, in terms of the unperturbed energy levels which are occupied by pairs of electrons up to the Fermi level and are empty above it. To simplify the discussion, we ignore the energy change due to the blocked states by unpaired electrons.

In 1D (as is the case here) the unperturbed energy will be reduced to: $\varepsilon_k = -2t \cos ka$ where a is the lattice constant. From the periodic boundary conditions, $ka = 2\pi j/N(-N/2 < j \leq N/2)$, and each energy level is degenerate for $\pm ka$ except for $ka = 0$ and π. Hence each level with $0 <\mid ka \mid< \pi$ can accommodate two pairs $(k\uparrow, -k\downarrow)$ and $-k\uparrow, k\downarrow)$. Thus when there are $4m+2$ electrons in the ground state, all the levels from $ka = 0$ up to $k_F a$ are fully

occupied by the pairs, while with $4m$ electrons, the Fermi level has a vacancy for one more pair. Therefore, when there are $4m$ electrons, a way to break a pair with minimum energy is to flip the spin of an electron of the pair at the Fermi level. The unpaired electrons then occupy the states $\pm k_F$ and there is no extra cost for the kinetic energy. On the other hand, when there are $4m+2$ electrons, one cannot break either pair at the Fermi level simply by flipping a spin, but an unpaired electron has to move up to the next available level, increasing the kinetic energy. This is why the E_{min} for pair breaking is larger for $4m+2$ electrons than for $4m$ electrons.

In the case of open boundary conditions or PBC with an impurity the degeneracy is broken so that E_{min} oscillates for every electron added to the system. One can observe that now the "frequency" of the oscillations has doubled and instead of peaks at $N_e = 4m + 2$ we have them at $2m + 1$. Interestingly the behavior of the system with impurities still differs from that with OBC. It was thought that the difference is because we should add an extra lattice point for the impurity site and so just a matter of different system sizes, N. However the difference persists with $N = 33$ for the impurity + PBC (with $V_{impurity} = 20t$). However the period and amplitude of oscillation for both OBC and the impurity + PBC are almost equal. The latter seems to be "pulled back" to lower energies.

Finally we found the Superconductor-Normal transition just by changing temperature and looking for the temperature region where Δ drops to zero. The BdG code, for cases with OBC and PBC works but there are problems with convergence of the method near the transition point, as is clear in Figures(3.9)-(3.12). E_{min} sometimes does not vanish for temperatures greater than the transition temperature, and even begins to increase again after a abrupt drop near T_c!.

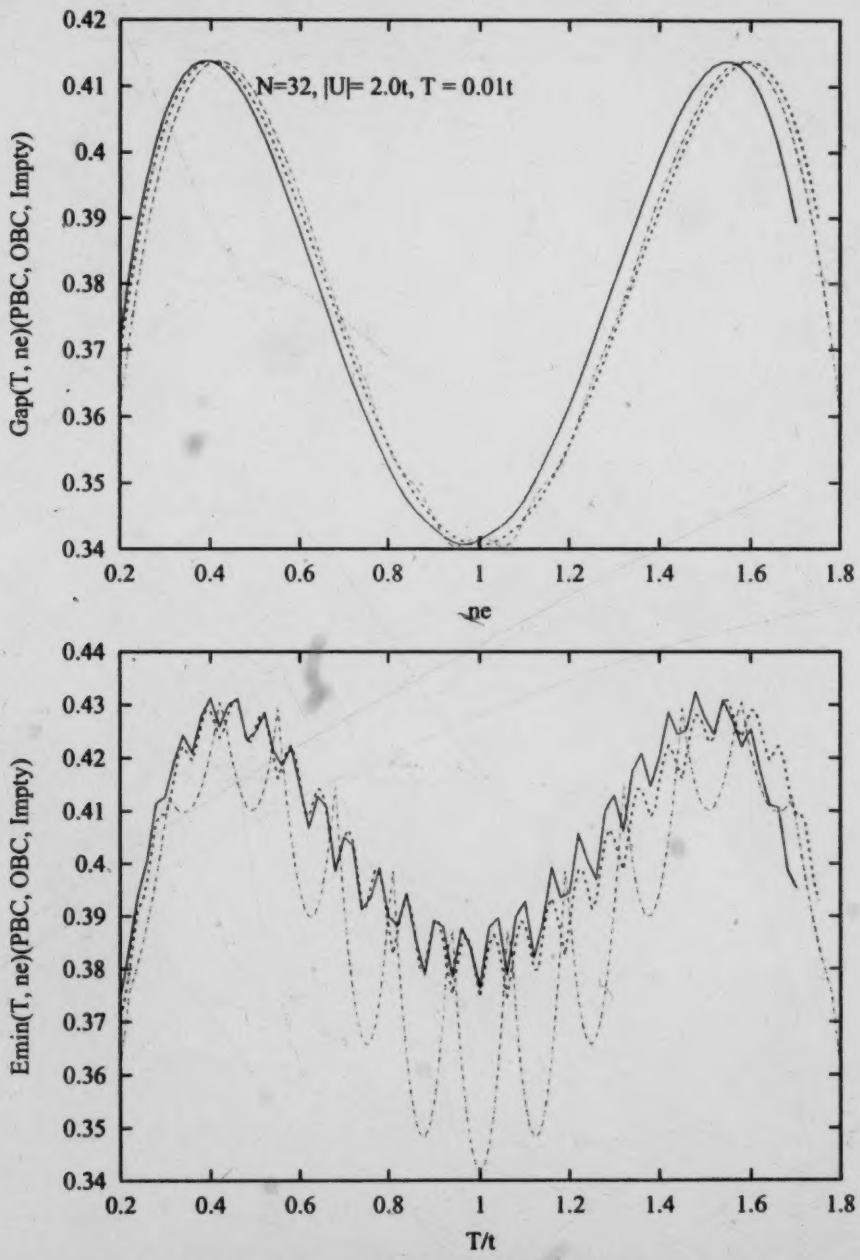

Figure 3.4: Results of PBC (dashed), OBC (light) and PBC with impurity (solid), (up) is the Gap function in the middle of the system and (down) the first excitation energy, E_{min}, for $|U| = 2.0t$, $T = .01t$ and $N = 32$ ($N = 33$ for PBC + impurity).

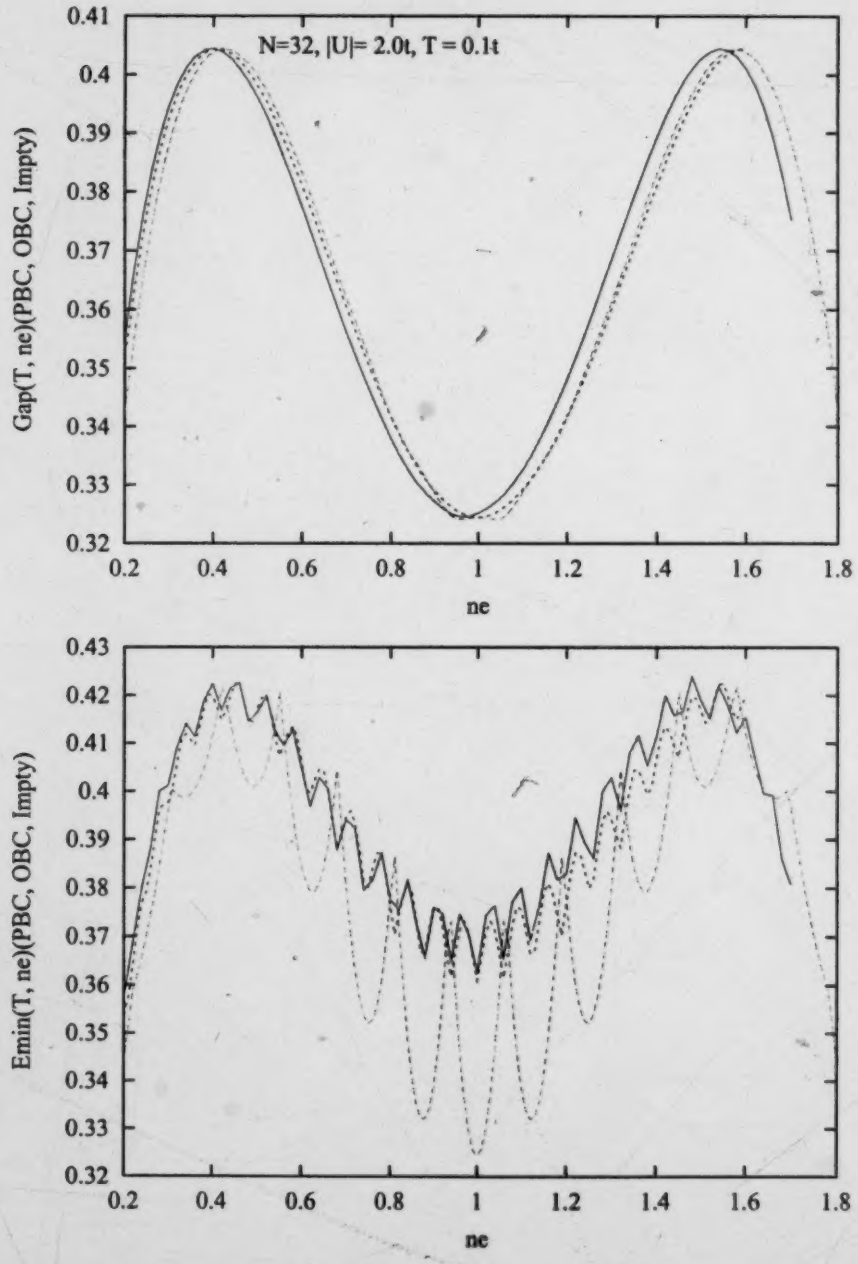

Figure 3.5: The same as FIG 3.4 for higher temperature, $T = 0.1t$.

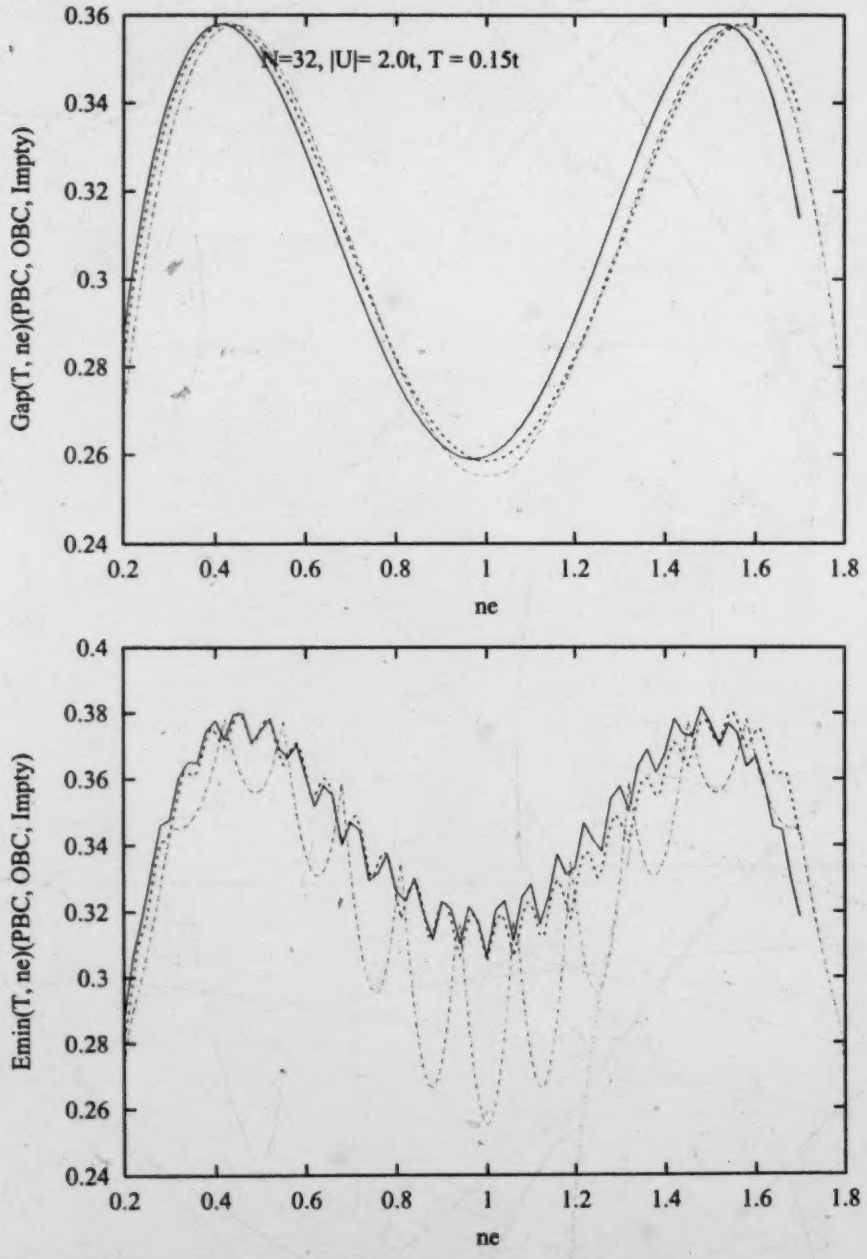

Figure 3.6: The same as FIG 3.4 for higher temperature, $T = 0.15t$.

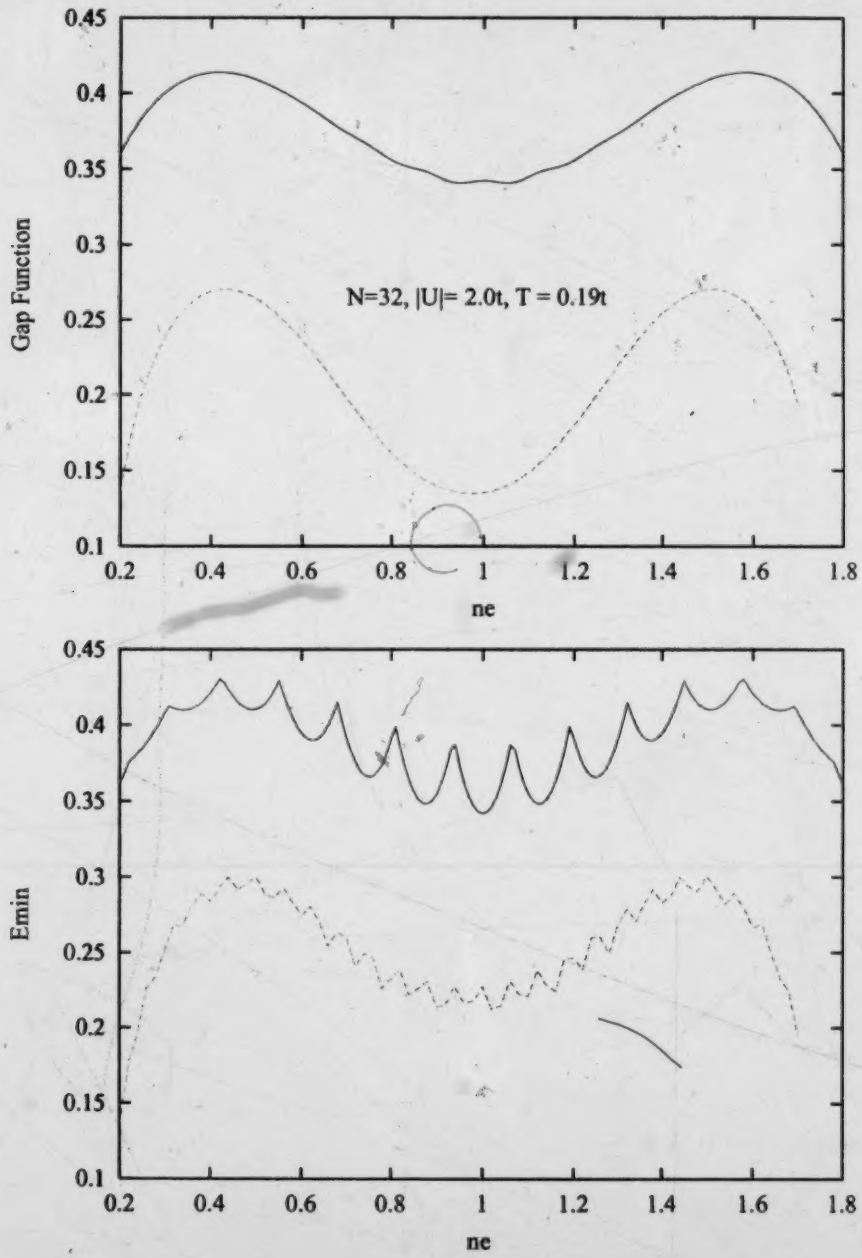

Figure 3.7: The same as FIG 3.4 with temperature close to transition temperature, $T = 0.19t$. The plots are for PBC (solid lines) and OBC (dashed lines).

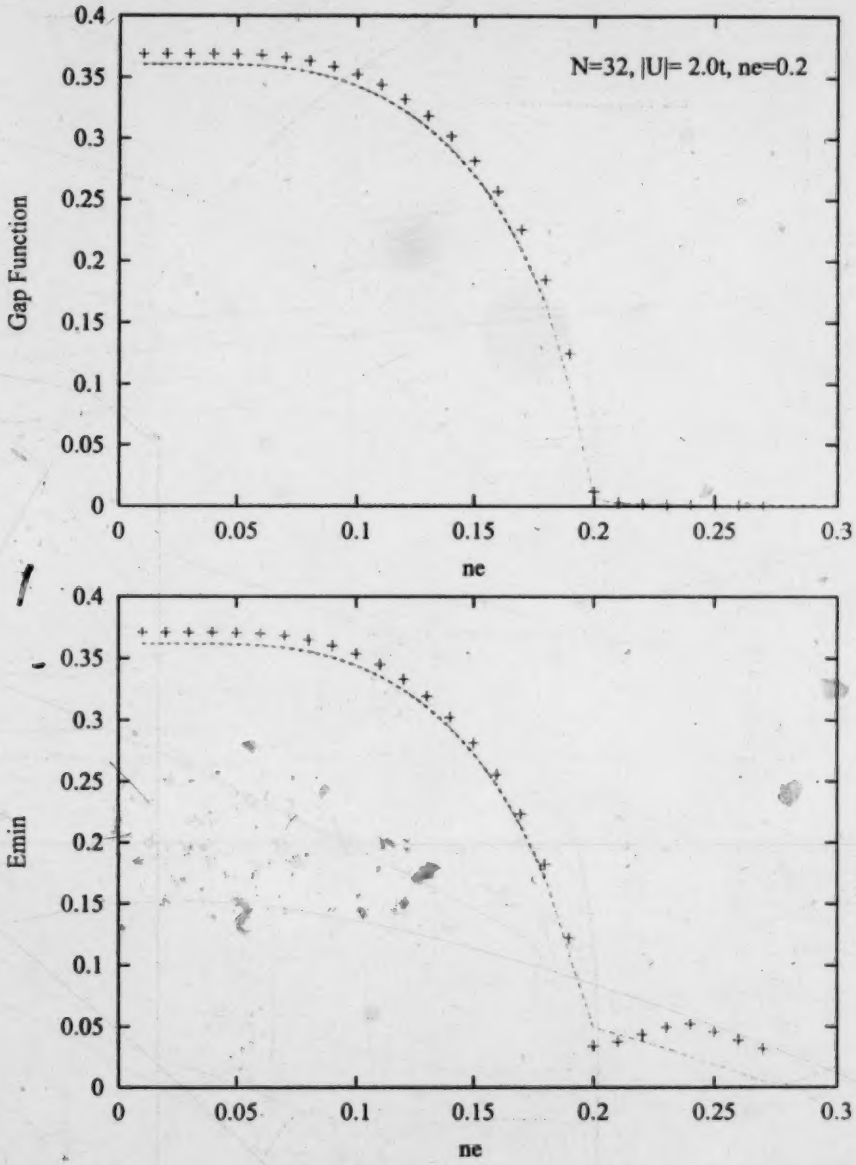

Figure 3.8: The temperature dependence of gap function in the middle of sysetm for BdG (light dashed lines) and BCS(dark dashed lines) and BdG with PBC (plus signs) (up). the same thing is plotted with first excitation E_{min}(down). for E_{min} the convergence near the transition $T_c \sim 0.2t$ is not enough accurate. $n_e = 02$ and $|U| = 2t$.

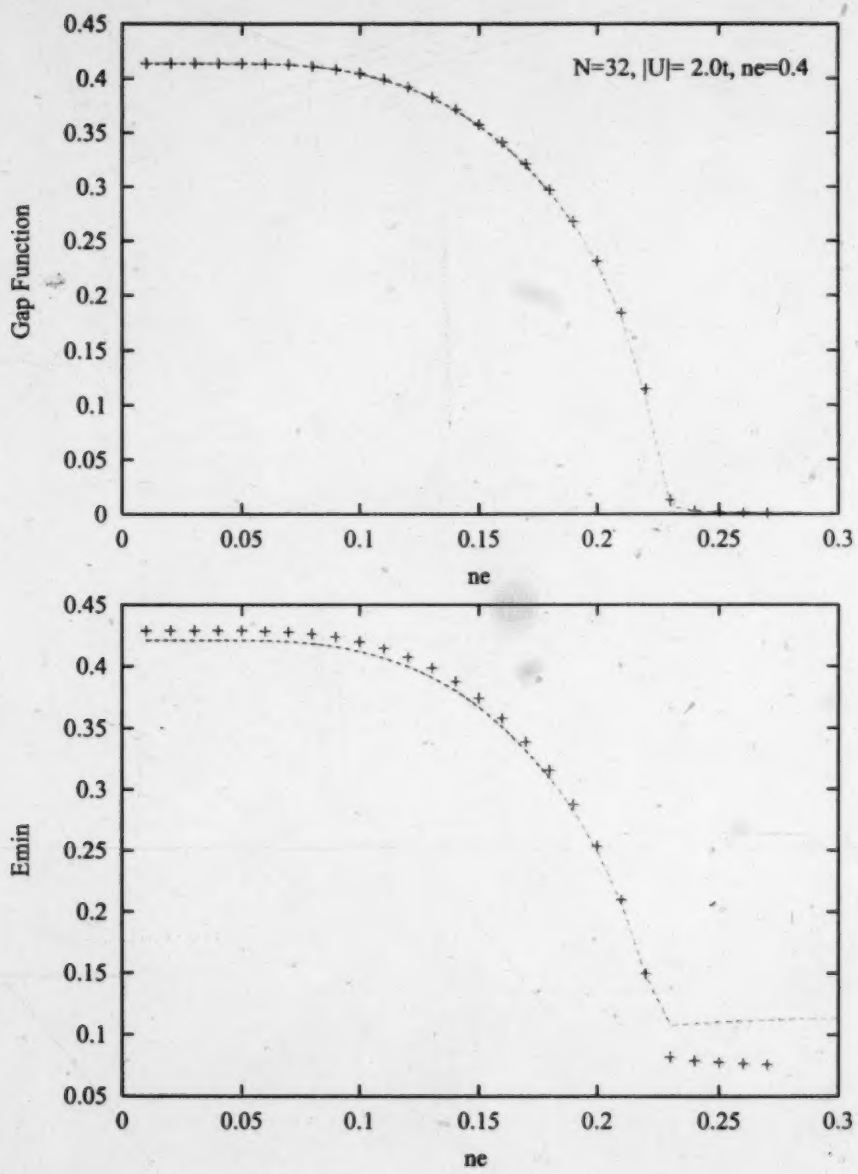

Figure 3.9: The same as FIG 3.8 for $n_e = 0.4$.

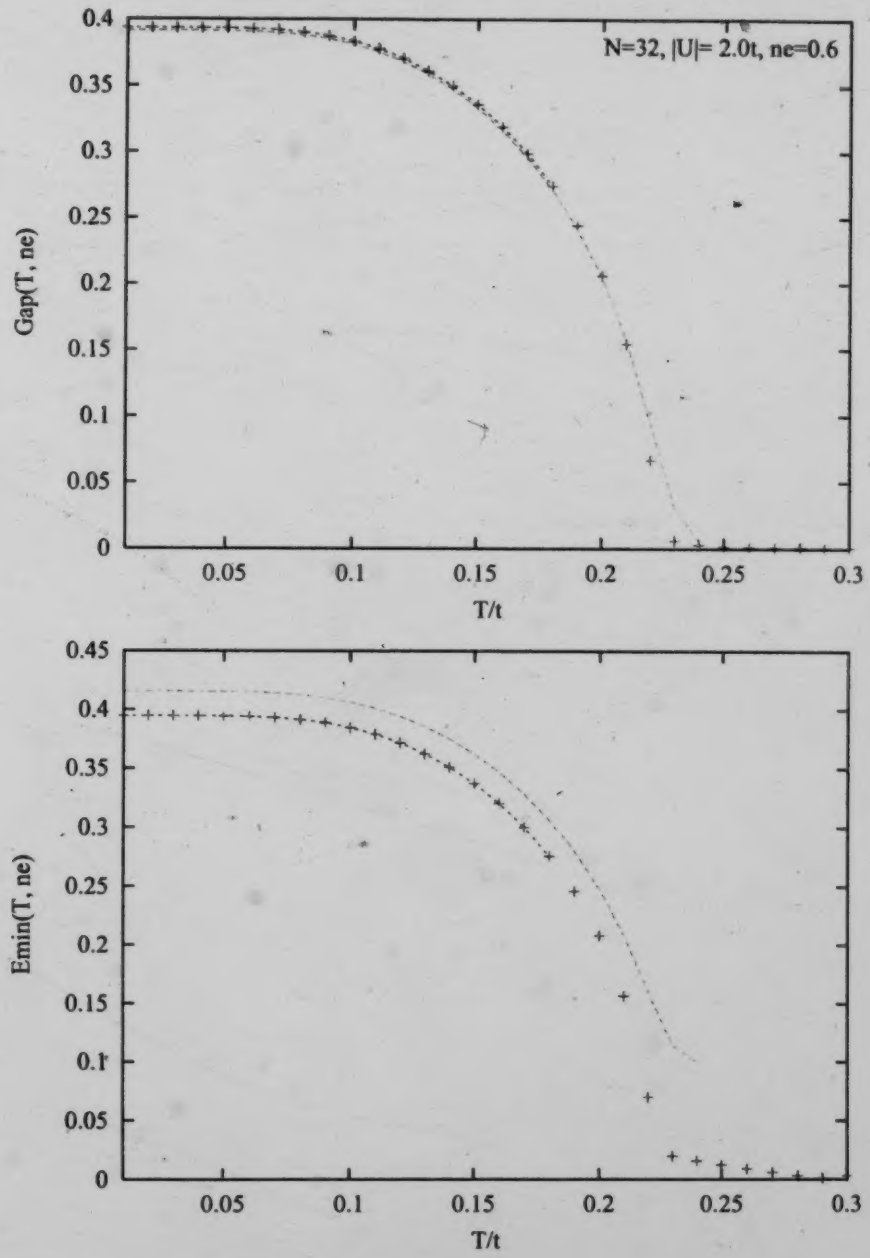

Figure 3.10: The same FIG 3.8 for $n_e = 0.6$.

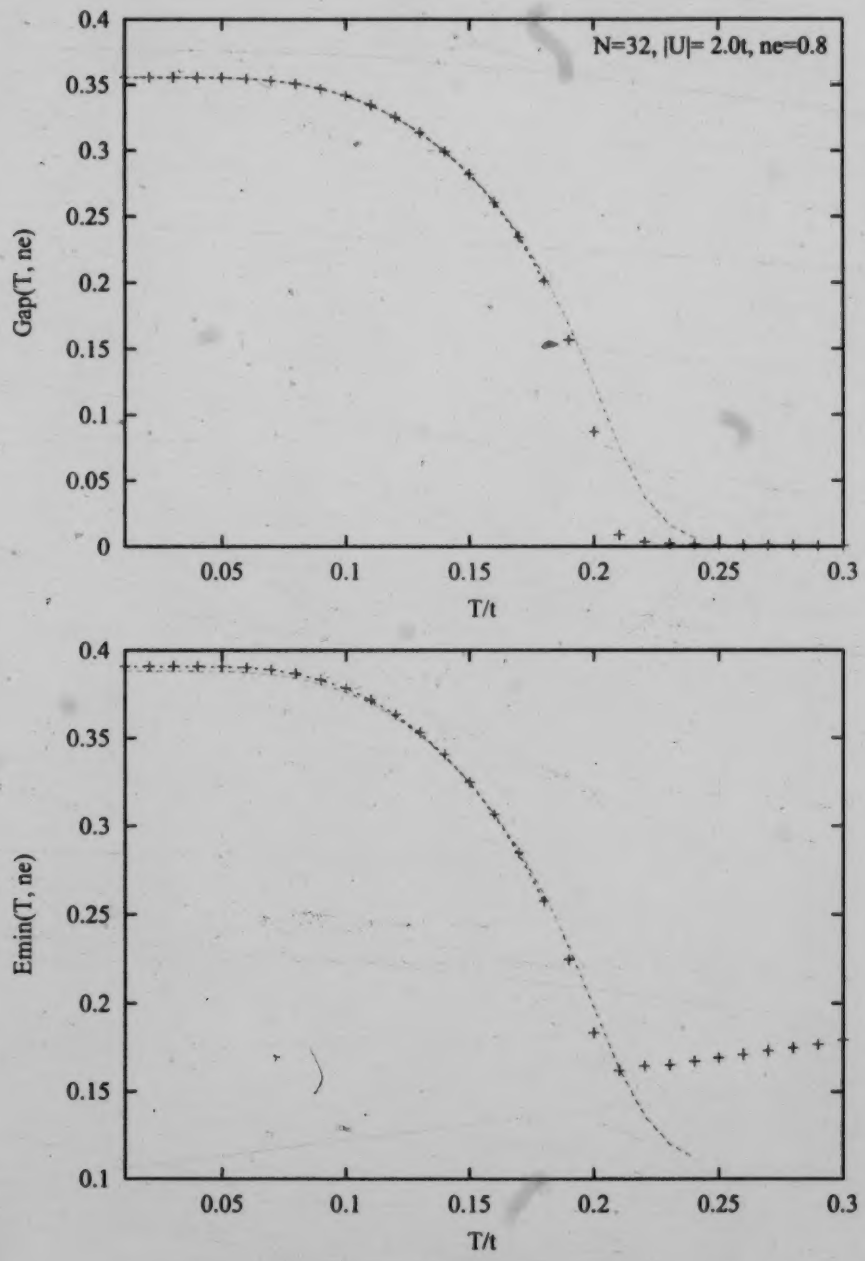

Figure 3.11: The same with FIG 3.8 for $n_e = 0.8$.

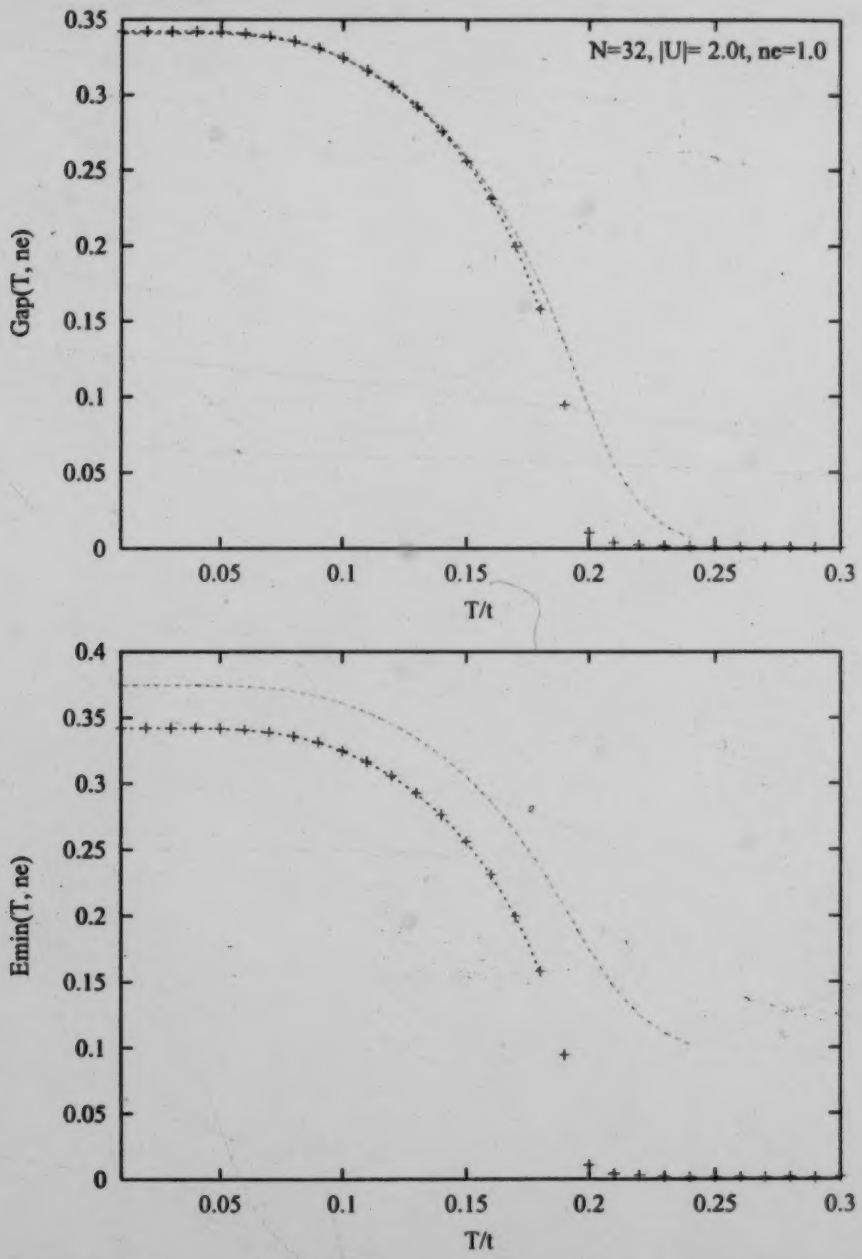

Figure 3.12: The same as FIG. 3.8 for $n_e = 1.0$. Note that in FIGs (3.9)-(3.13) the $\Delta_{bulk}(T = 0.01t)$ is oscillating with the change of n_e as we expect from FIG 3.4.

3.6 Spatial behaviour of gap function

One of the main goals for considering finite-size systems is to see the self-consistent solutions of the gap function as a function of coordinate near the boundaries, in a more general sense than what Landau-Ginzburg theory presents [2], since at the microscopic level LG is not appropriate. The results obtained below generally show sensitivity to the electron filling parameter, n_e, though only implicitly to Hubbard interaction strength U, or the system size, N. As we expect the solutions go to a constant in the middle of the system even for fairly small systems (typically for U fixed at $2t$). This constant $\Delta_{N/2}$ is different from that of BCS for small system sizes like $N = 32$; however, it converges to the same value as we increase the system size. For $N \geq 256$ it agrees with the BCS gap value within numerical errors.

Before we discuss the solutions for Δ_i, we should examine the wave-functions for typical values of the parameters , $|U| = 0.5$, $T = 0.01t$ and a large system $N = 256$. First and second excitations are plotted in FIG.s(3.13) and (3.14). It is not surprising that for particles and holes we have a standing wave, as the system has a confined geometry. In FIG.(3.15) we plot the gap as a function of position, there we observe dominant, *non-zero* terms near the boundaries (the reason for choosing a weaker $|U|$ ($|U| = 0.5t$) than the previous case ($|U| = 2.0t$) is that with weaker coupling the variation of gap can be seen over a wider range, i.e. the resolution is higher).

For $n_e = 0.2$, FIG. (3.16) shows that Δ_i goes to zero as we approach the boundaries as intuitively expected. There is also a maximum in the gap value near the boundaries, a feature also present in the quasi-classical calculations [39]. However, to the knowledge of the writer there is no formal relation between the quasi-classical approximation and the BdG equation in this regime ($n_e \ll 1$) . In fact one might expect the opposite, since, for $n_e \ll 1$, the Fermi surface no longer

dominates; this is reminiscent of strong-coupling limit where the quasi-classical approximation is no longer valid.

The distance from boundaries over which Δ_i changes appreciably is not size-dependent nor dependent on n_e as can be seen by comparing the upper result ($n_e = 0.2$) with the lower one ($n_e = 1.0$) in FIG (3.16). However there is a strong dependence on $|U|$ (since the range over which Δ_i varies is about the correlation length, which is determined by the pairing strength.

A different regime that is interesting is near half filling, $n_e \sim 1$. The gap function increases in amplitude and oscillates as we approach the boundary, as has been reported in the literature directly [6], [26] and indirectly [40]. As mentioned above it basically comes from the fact that we are solving the Bogoliubov-de Gennes equations self-consistently and since for a self-consistent solution you should encounter all different frequencies, for big Fermi surfaces (i.e., $n_e \sim 1$) we expect to see the effect of high frequencies as oscillations in Δ_i near the boundaries.

Decreasing $|U|$ results in a larger correlation length, so, as may be expected, the oscillations will go much further inside the system for $U = 0.5t$ as shown in FIG.(3.16), though still the half-filling one is much more significant, the similarities between the FIG.(3.16)(up) and [6] is noticeable.

In the next step, we checked the behavior of Δ near an impurity and a boundary. The corresponding graphs are plotted in FIG.(3.17)(up). The two results look similar, but they are shifted (again we expect this since the graphs of Δ in previous FIGs (3.4)-(3.8) was also shifted. The pairing strength was chosen not to be large ($|U| = 1.0t$) and the system size was chosen to determine well converged results.

It is interesting to observe the behavior of the gap both with respect to coordinates and temperature FIG(3.18) or electron density FIG(3.19). For half-

filling the gap function does not have a smooth hyperbolic tangent form, or anything similar and becomes almost a hyperbolic tangent at the boundary near $T \sim T_c$. This is in agreement with the quasi-classical approximation, but in that case no information about n_e dependence is available.

We should emphasize the surprising behavior of the gap at the boundary for $n_e \ll 1$, $\Delta(i=1) = \Delta(i=N) \neq 0$ and for $n_e \sim 1$, $\Delta(i=1) = \Delta(i=N) \gg \Delta_{Bulk}$. This is because of the discrete nature of the problem: the sites $x = 1$ and $x = N$ are not exactly the "Boundary" points and we expect an abrupt change in the gap function to zero as mentioned in [6] for both cases.

The oscillatory solutions for Δ_i can be understood by checking the number of $u_{n,i}v^*_{n,i}$ terms that are required to reach a good self-consistent solution (recall that for the case of the quasi-classical solutions near $T \sim T_c$ it was only the first two leading terms that were included). In the case of low filling, only afew terms were needed to satisfy self-consistency, but near half-filling most of the terms were required to be able to observe the self-consistent oscillatory behavior.

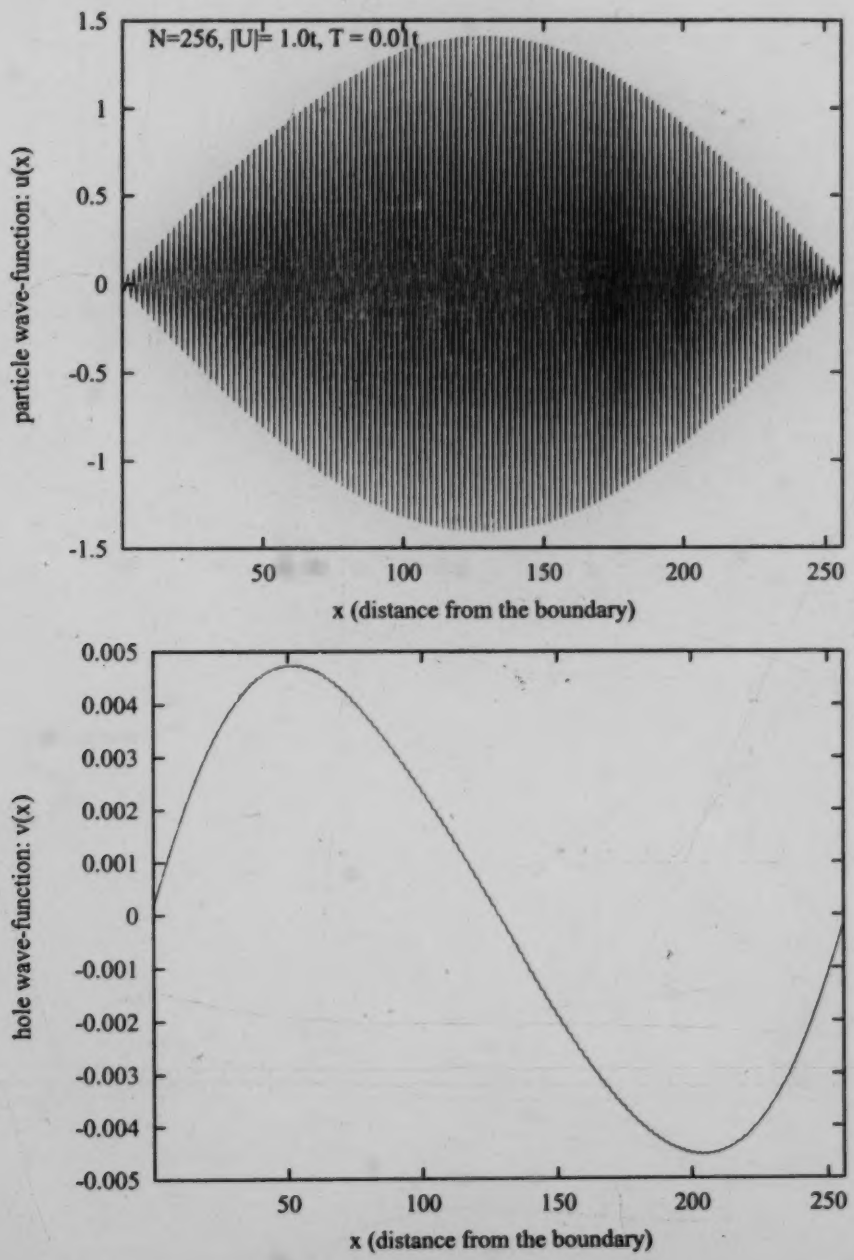
N=256, |U|= 1.0t, T = 0.01t
particle wave-function: u(x)
x (distance from the boundary)
hole wave-function: v(x)
x (distance from the boundary)

Figure 3.13: A typical wave-function (Bogoliubov amplitudes u_n and v_n), for $n = 1$, particle wave-function(up) indicates u_n and hole wave-function (down) indicates v_n, the system size is fairly large to show the spatial variations of wave-functions better.

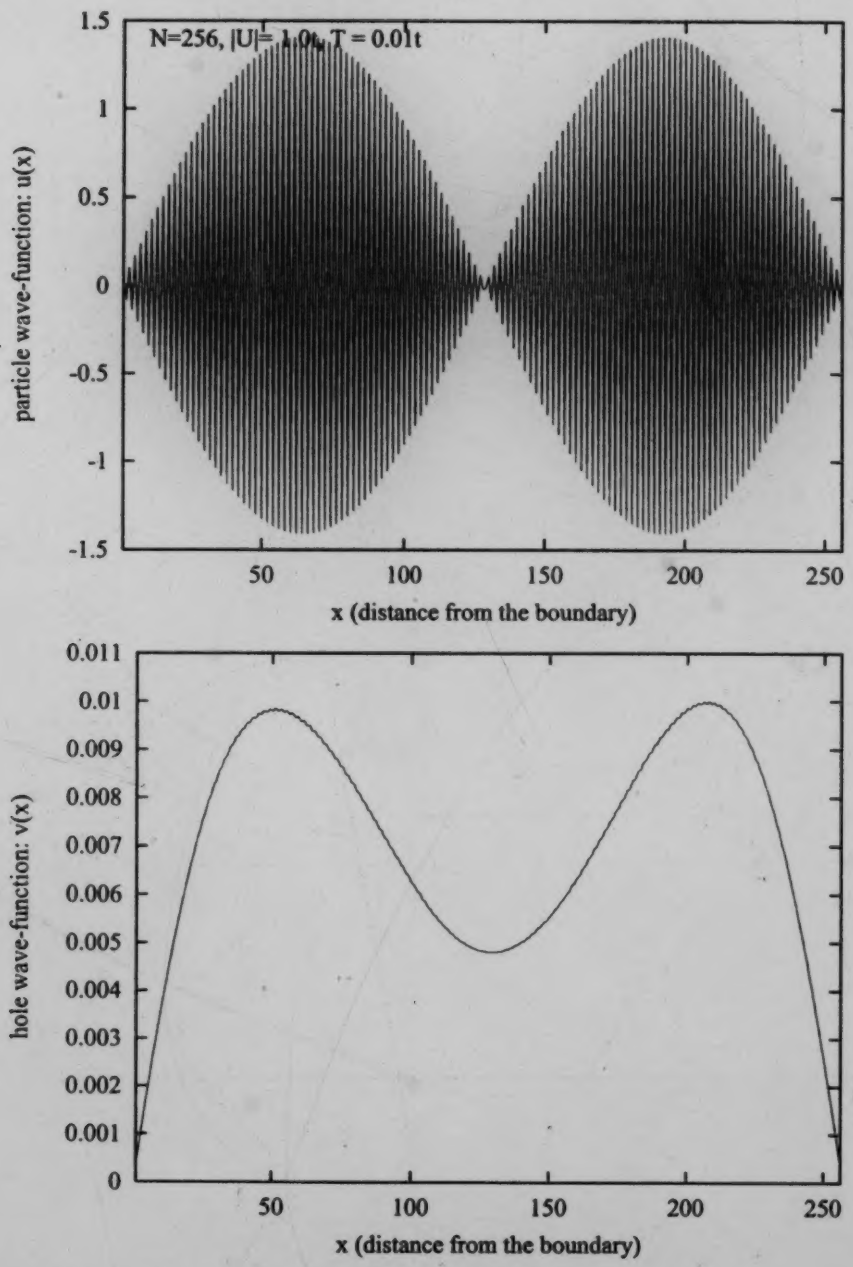
N=256, |U|= 1.0t, T = 0.01t
particle wave-function: u(x)
x (distance from the boundary)
hole wave-function: v(x)
x (distance from the boundary)

Figure 3.14: The same as FIG. 3.13, but for the second excitation, $n = 2$, notice the parity changes of v_n, (as we expect).

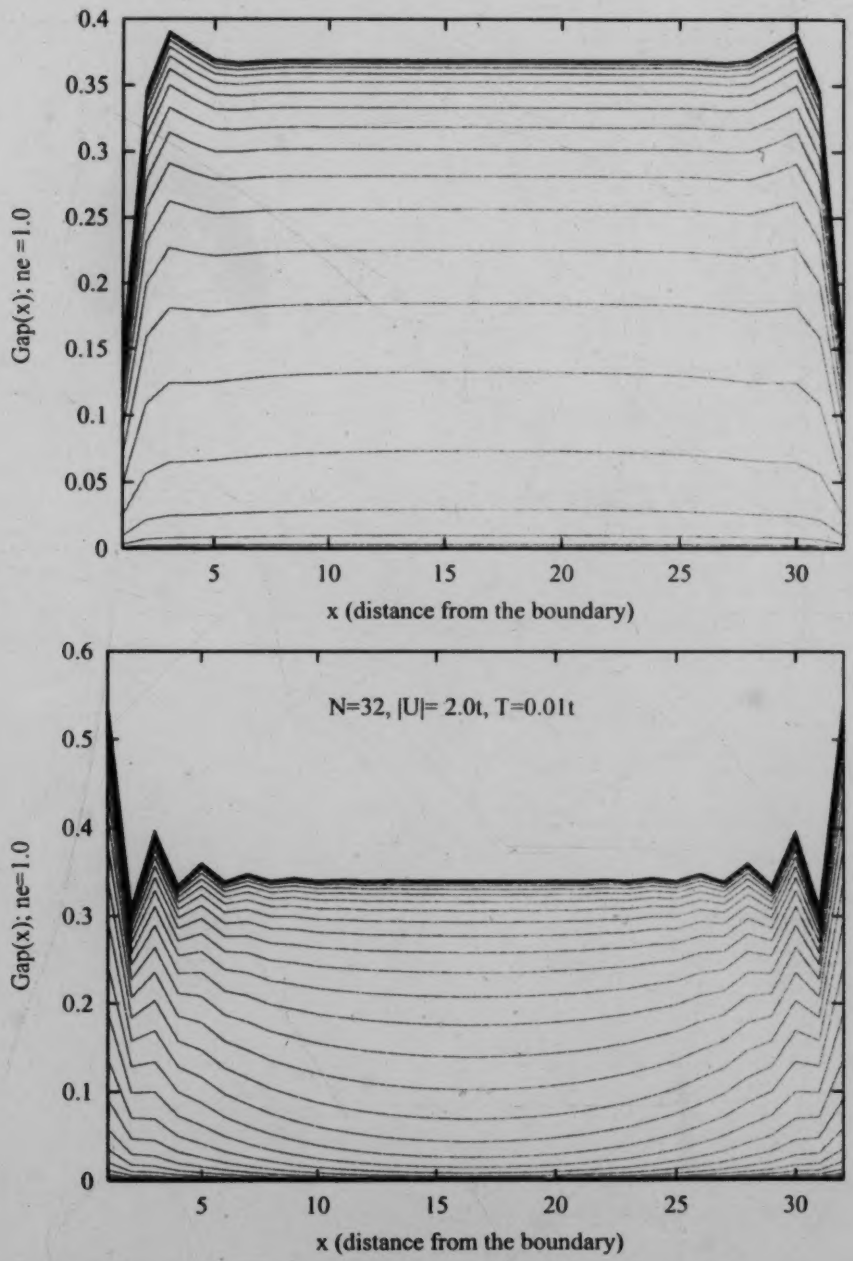

Figure 3.15: Profile of $\Delta(x)$ for different temperatures. (up) is the low n_e regime that behave like quasi-classical solutions and goes to a smooth hyperbolic tangent near transition as expected. (down) in half-filling the gap oscillates near the boundaries the oscillations vanish as we approach the transition point, but we do not recover the hyperbolic tangent behavior.

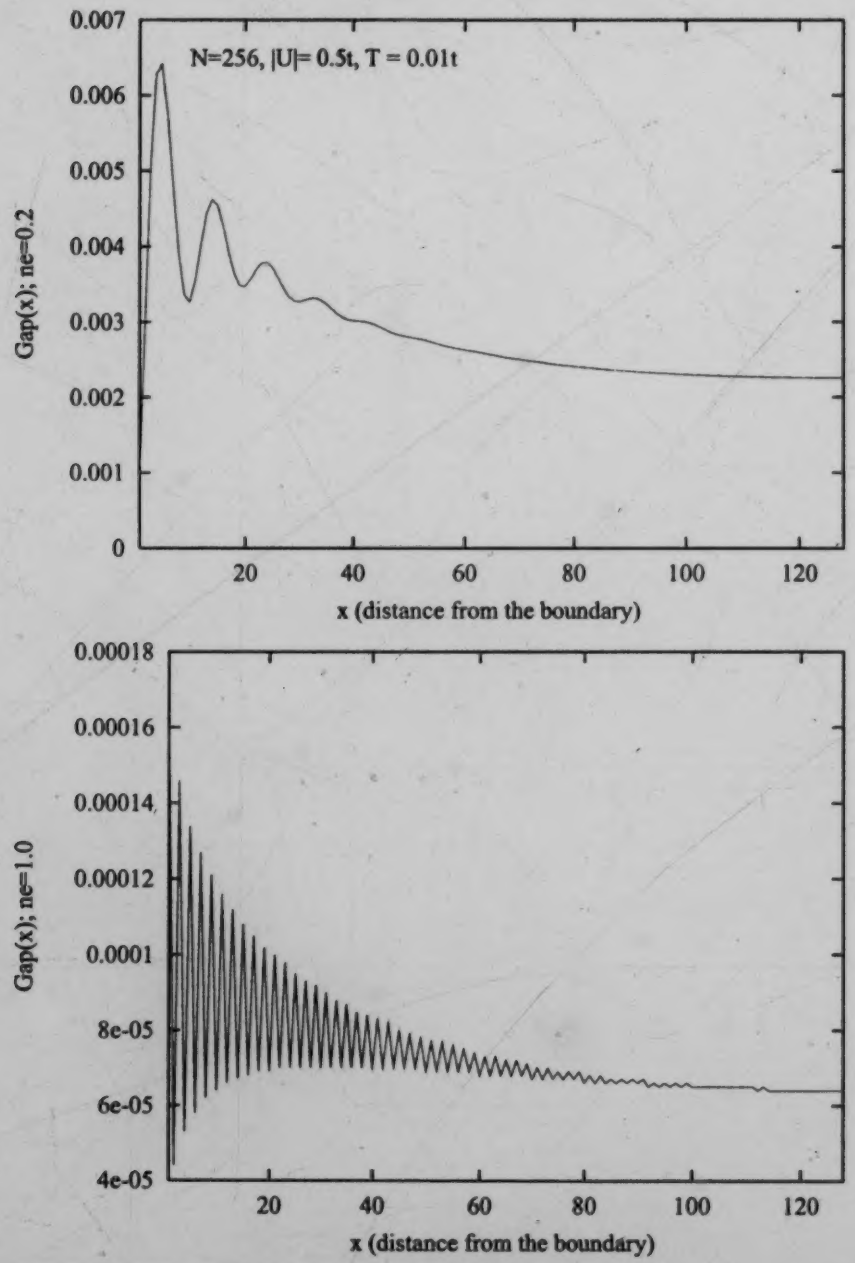

Figure 3.16: The same thing for smaller pairing strength, $|U| = 0.5$ and bigger system sizes (to achieve convergence, also having the appropriate gap (since the oscillations will penetrate more than 32 sites inside the system). (up) zero temperature ($T = 0.01t$) and low n_e, $= 0.2$. (down) zero temperature and half filling.

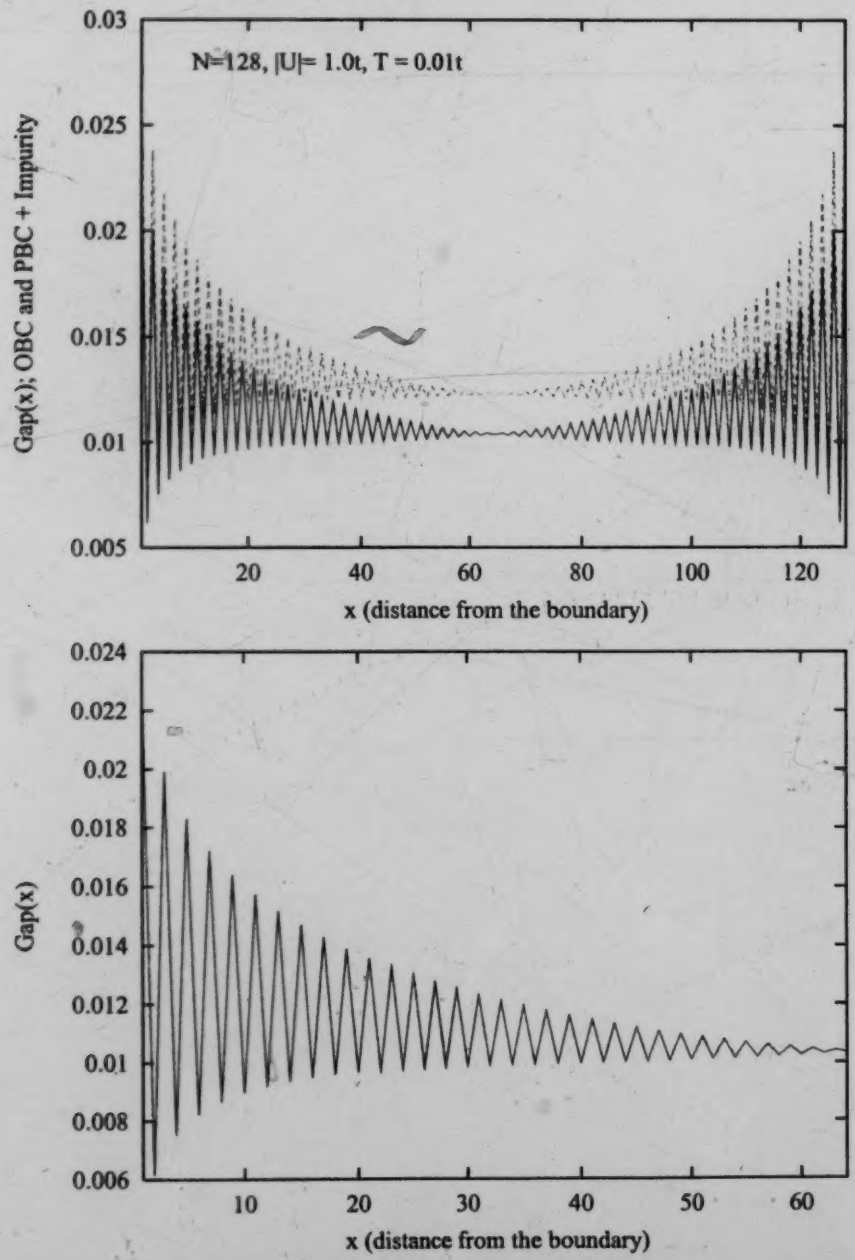

Figure 3.17: Comparison of the PBC with impurity on the side with the tight-binding model(OBC), for $|U| = 1.0t$ and , $n_e = 1.0$ and $N = 128$ (fairly large). (up) is the whole graph (solid is the OBC) and (down) is the OBC one magnified near the boundary.

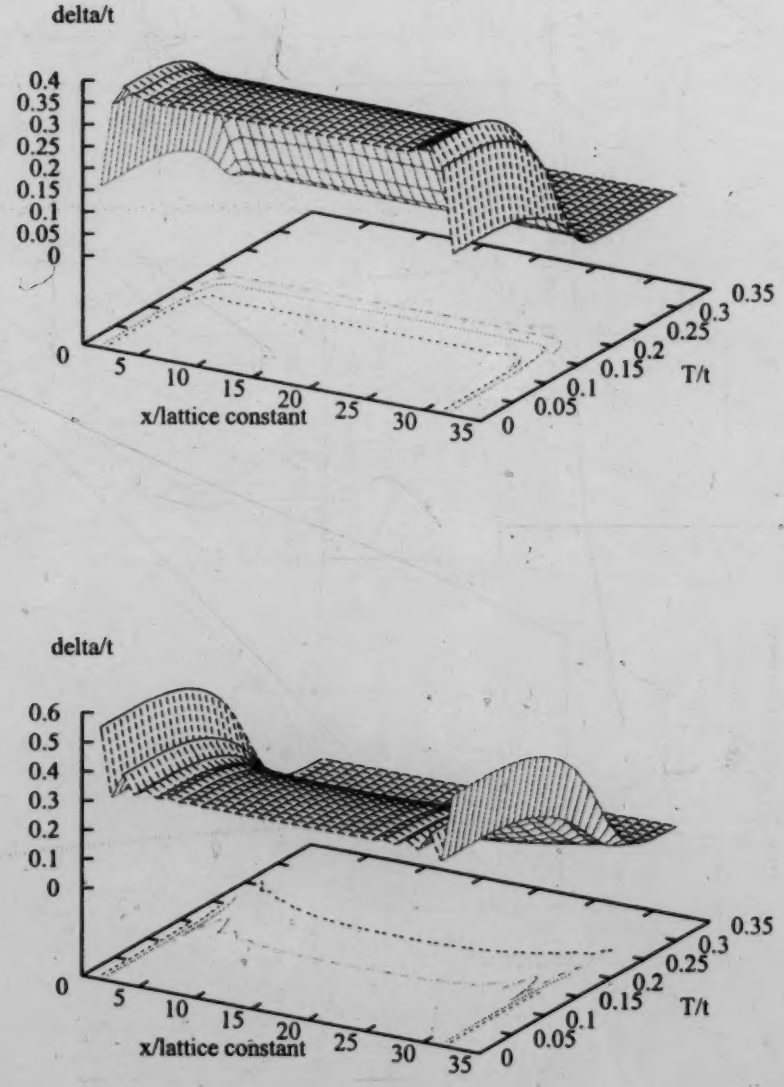

Figure 3.18: The two-dimensional graph of $\Delta(x)$ vs. Temperatures, for two different electron densities, $n_e = 0.2$ (fairly low-filling) (up), $n_e = 1.0$ (half-filling) (down).

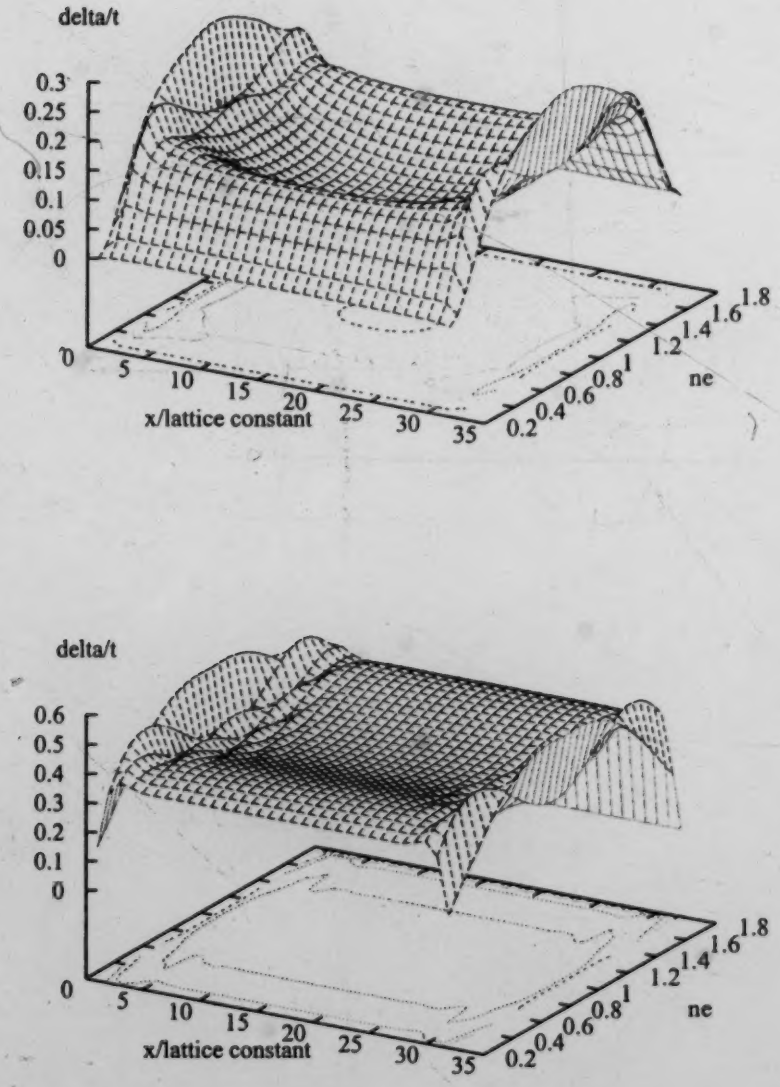

Figure 3.19: The two-dimensional graph of Δ_i vs. n_e, for two different temperatures, $T = 0.19t$ (near transition) (up), $T = 0.01t$ (zero temperature) (down).

3.7 Local Density Of States(LDOS)

Since the availability of STM techniques to probe the local density of states of superconductors on their surfaces and since the DOS of the BCS theory is well-known and understood, we have two possibilities to check our LDOS results obtained through self-consistently solving BdG in these two extremes: surfaces and in bulk. But, first of all let us write the more general formula for LDOS in the presence of the non-homogeneous system (specially when there is no particle/hole symmetry) as,

$$\mathcal{N}(E,i) = \sum_n (\mid u_{n,i} \mid)^2 \delta(E - E_n) + (\mid v_{n,i} \mid)^2 \delta(E + E_n) \tag{3.20}$$

that can be understood by noting that $u_{n,i}$'s are the amplitude for quasi-particles and respectively $v_{n,i}$'s for quasi-holes (that since holes correspond to the minus sign energies, the + sign appears in the second $\delta-$function).

To make the calculations possible to do with a computer I use a Lorentzian form for $\delta(y)$, i.e., the identity:

$$\delta(y) = \lim_{\Gamma \to 0} \frac{1}{\pi} \frac{\Gamma}{y^2 + \Gamma^2} \tag{3.21}$$

Approximating $\delta(E \pm E_n)$ in equation (3.20) with a Lorentzian form with a finite value for Γ we can minimize finite system-size effects, since Γ broadens the shape of the δ-function and it may make the final LDOS obtained continuous. This is really needed especially for small lattices but since with broadening the δ-functions we are also losing some of the bare information (that may be quite important). I also increase the system size by a factor of 10 (instead of 32 sites, typically, for LDOS calculations it is 256) and fix the value of Γ ($\Gamma = 0.04$).

In all the FIGs, from Fig(3.20)-(3.31), the most important observation is that *because* of finite size, the LDOS inside the system, shows an oscillatory

behavior and it smoothen as we approach the middle of the system and in the middle we recover the BCS result (in this case it is somewhat artificial, since I chose Γ so that we get the BCS result in bulk). The typical picture is that for sites right near the boundary we have a kind of "surface state' and their form of LDOS is totally different than what is inside. Then with every step toward the middle of the system the LDOS gets two more peaks and after about 10 sites (this number depends on the correlation length, i.e., pairing strength) we begin to observe the BCS divergences in the LDOS. This is accompanied with a strong oscillation in the energy range between -1.5t to 1.5t, roughly, for both the superconducting and the normal metal case. Recovering the BCS result in the middle of the system (sites 128 and 129) i.e., absence of these oscillations, will confirm that they are a finite size effect of the system. Actually this has been observed experimentally before [30]. There is also a recent theoretical work based on solutions of Gor'kov equations [29]. Rowell et. al. call it the "Superconducting version of Friedel oscillations", but to the author it is not clear what the relation of Friedel Oscillations (that are basically spatial) is to LDOS oscillations (for Friedel oscillations c.f. [37]).

It should be mentioned that because of the high value of the smoothing parameter I chose (since I wanted to distinguish between effects of discrete system and finite sizes) the gap width cannot be seen as is theoretically predicted. Especially on the surface LDOS in the second site, it is hardly distinguishable from the normal LDOS.

Also the other interesting observation is that the width of the gap that can be seen from LDOS near zero energy, is not in accordance with the results we got from our spatial behavior of Δ_i, in the previous section when we were considering the spatial behavior of the gap function. We could see that there are strong oscillations near the boundaries (at least for half-filling it was quite clear) but just

looking at the gap that can be seen from the surface DOS and the corresponding one far inside the superconductor we cannot see much difference, as opposed to the huge changes for Δ_i near the boundaries. This is actually in agreement with STM experiments that confirm a gap of the order of the BCS energy gap using surface measurements [7]. Also the same remarks apply to the ARPES experiments (Angle Resolved Photo Emission Spectroscopy)[24, 25]

As can be seen from Figs (3.21)-(3.28), the effect of changing the electron density is basically a shift in the whole shape of the LDOS diagram, but having the gap around zero energy as we expect it to be, this is qualitatively in agreement with the BCS results we are accustomed to already.

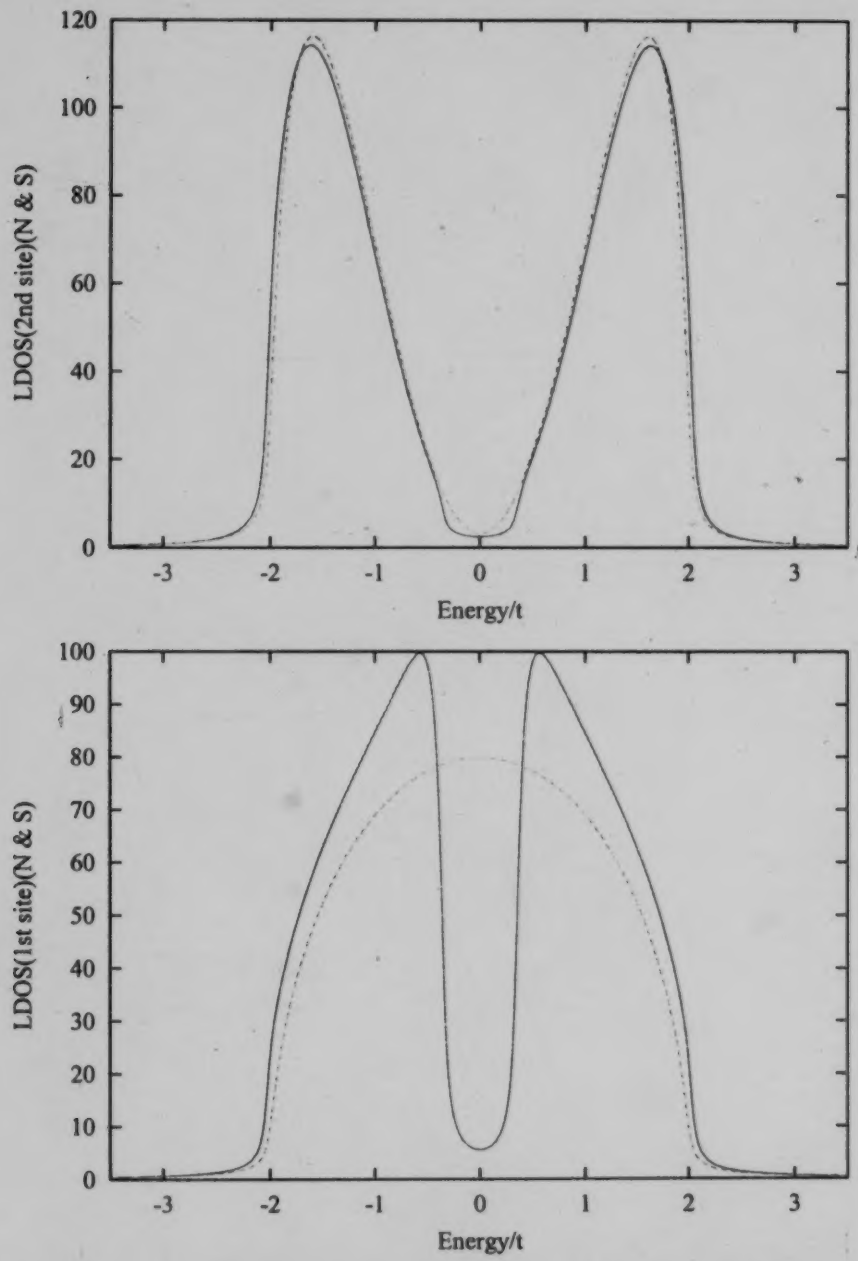

Figure 3.20: Local density of states(LDOS) for 256 site system at the first(down) (up) sites, at zero temperature($T = 0.01t$), $n_e = 1.0$ and $|U| = 2.0t$. The solid lines are normal metal and dashed lines are superconducting solutions.

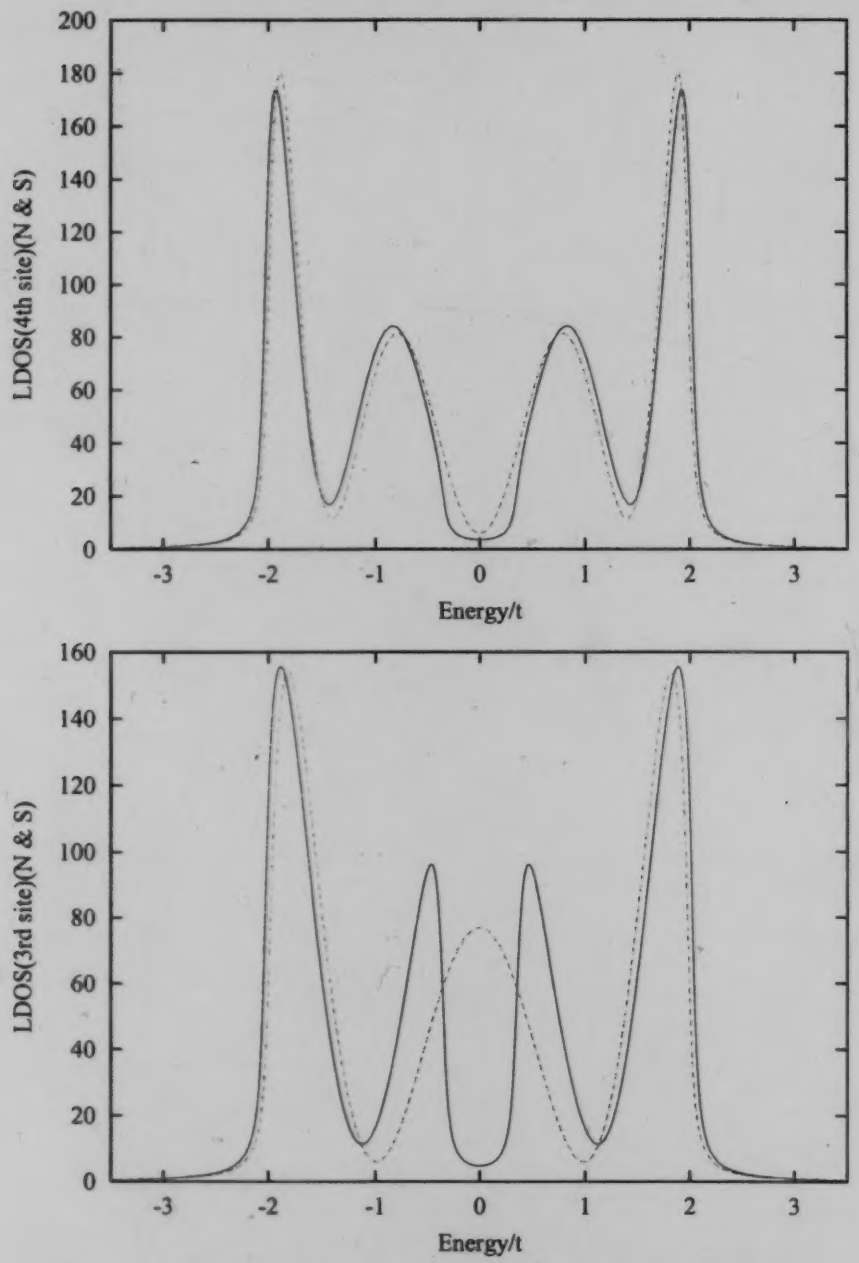

Figure 3.21: The same as FIG. 3.20 for third(down) and fourth(up) sites.

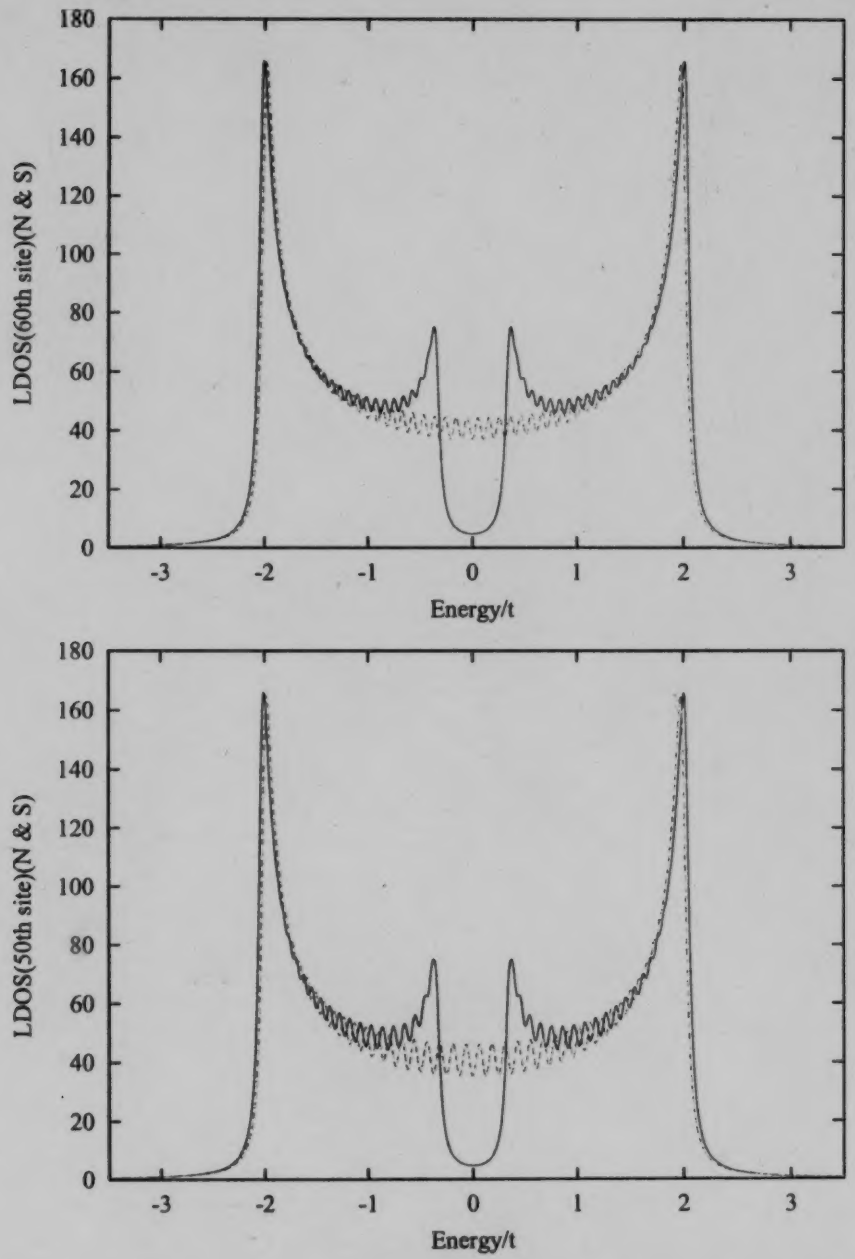

Figure 3.22: The same as FIG.(3.20) for 50th(down) and 60th(up) sites.

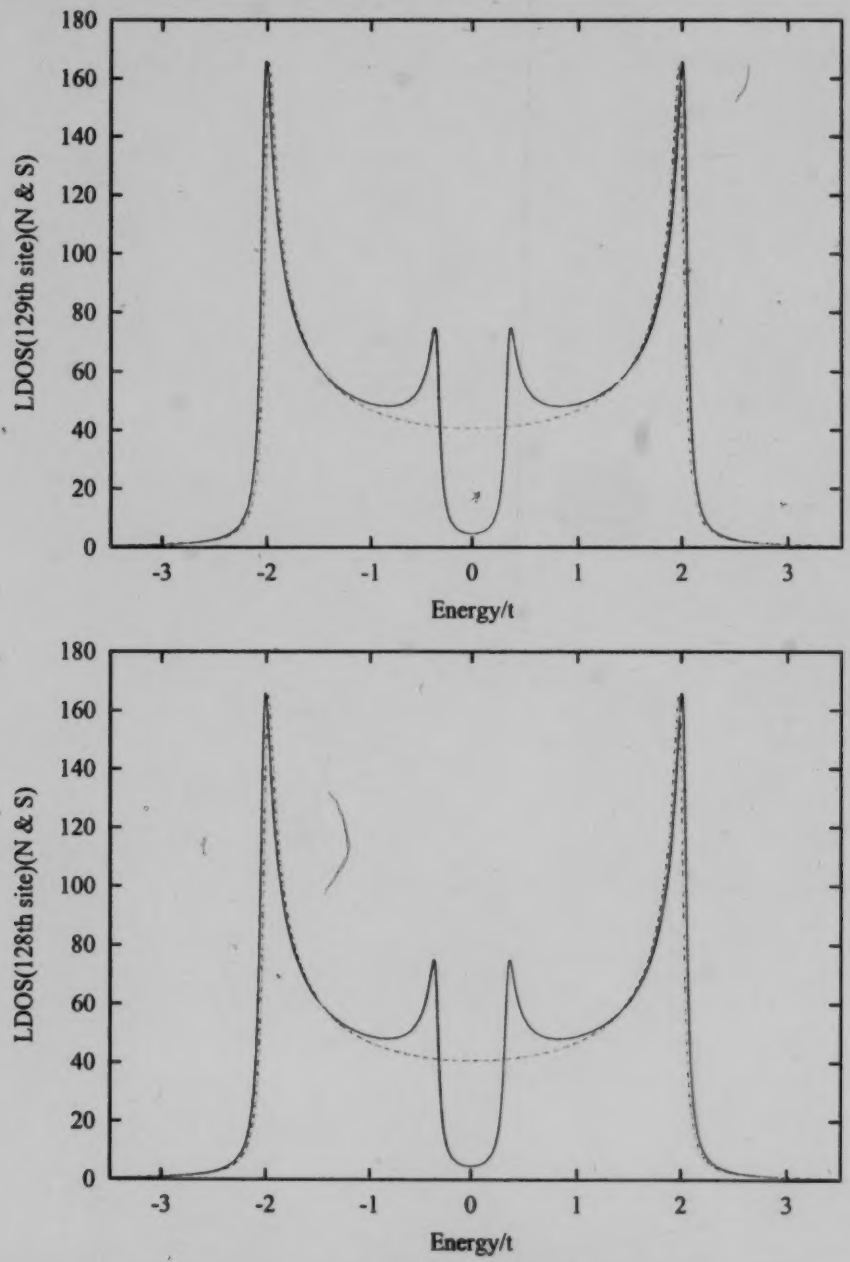

Figure 3.23: The same as FIG.(3.20) for 128th(down) and 129th(up) sites. It is exactly the middle of system, and as can be seen the oscillations in LDOS almost vanish and we recover the BCS DOS form. Note that for $n_e = 0.2$ we would have the mirror reflection of the above graphs around $E = 0$ axis.

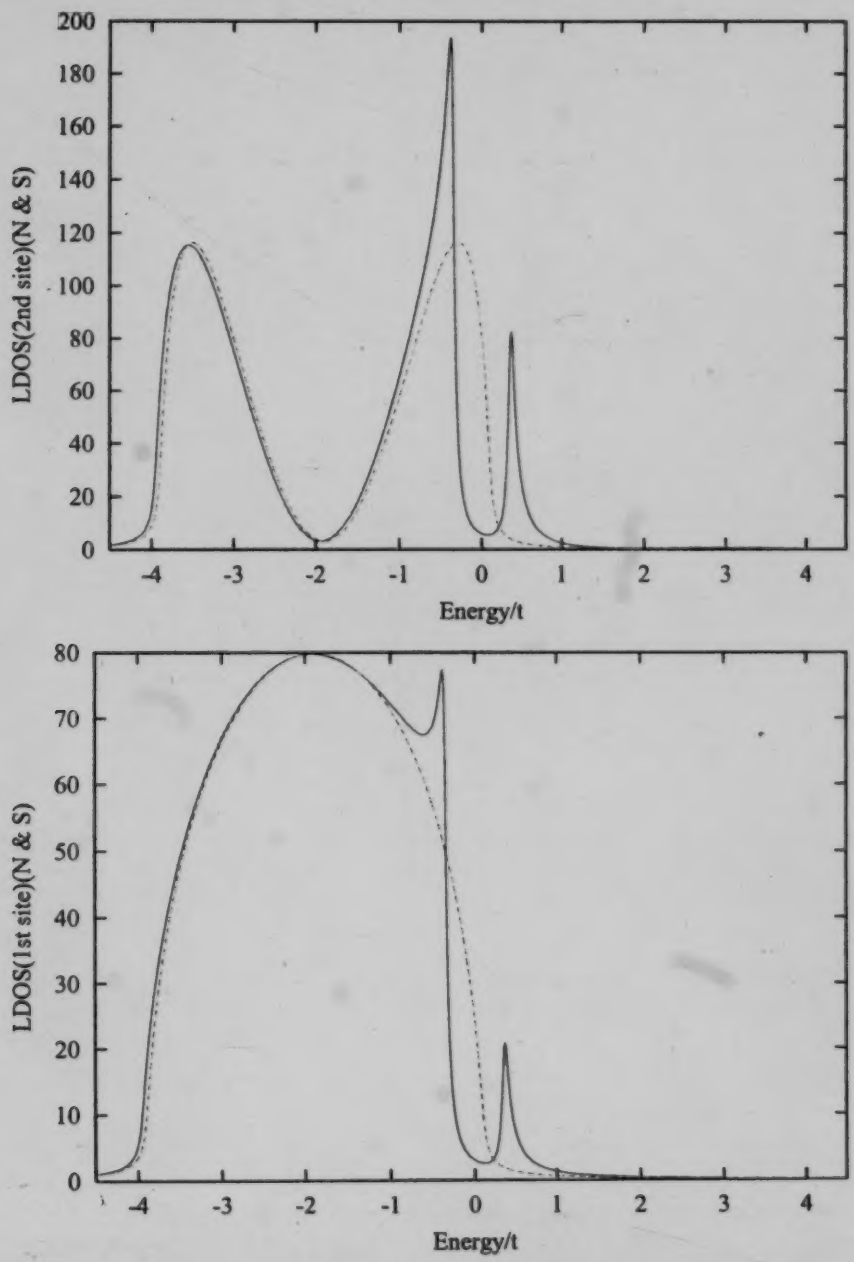

Figure 3.24: Local density of states(LDOS) for 256 site system at the first(down) and second(up) sites, at zero temperature ($T = 0.01t$), $n_e = 1.8$ and $|U| = 2.0t$. The solid lines are normal metal and dashed lines (again notice that we will have the same curves for $n_e = 0.2$ just mirror reflected around $E = 0$).
are superconducting solutions.

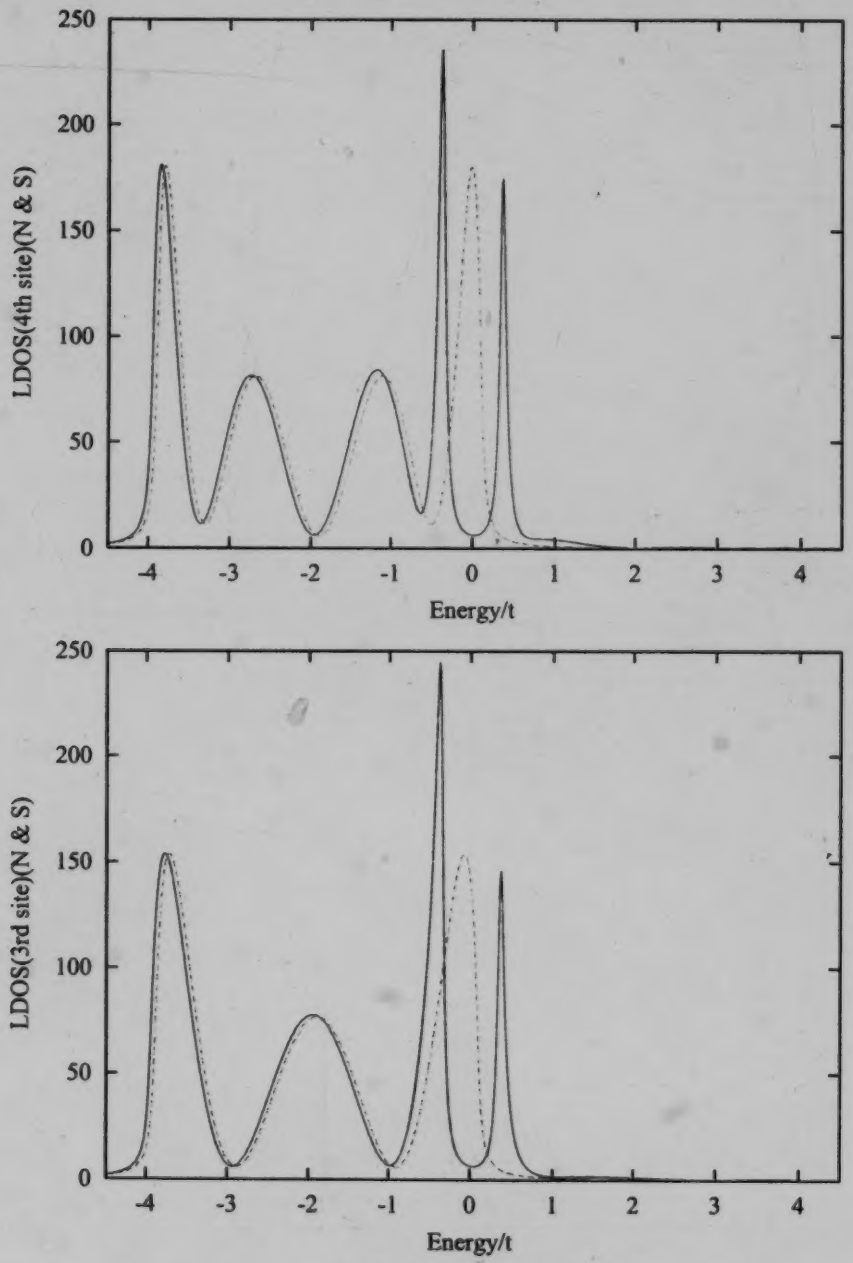

Figure 3.25: The same as FIG.(3.24) for third(down) and fourth(up) sites.

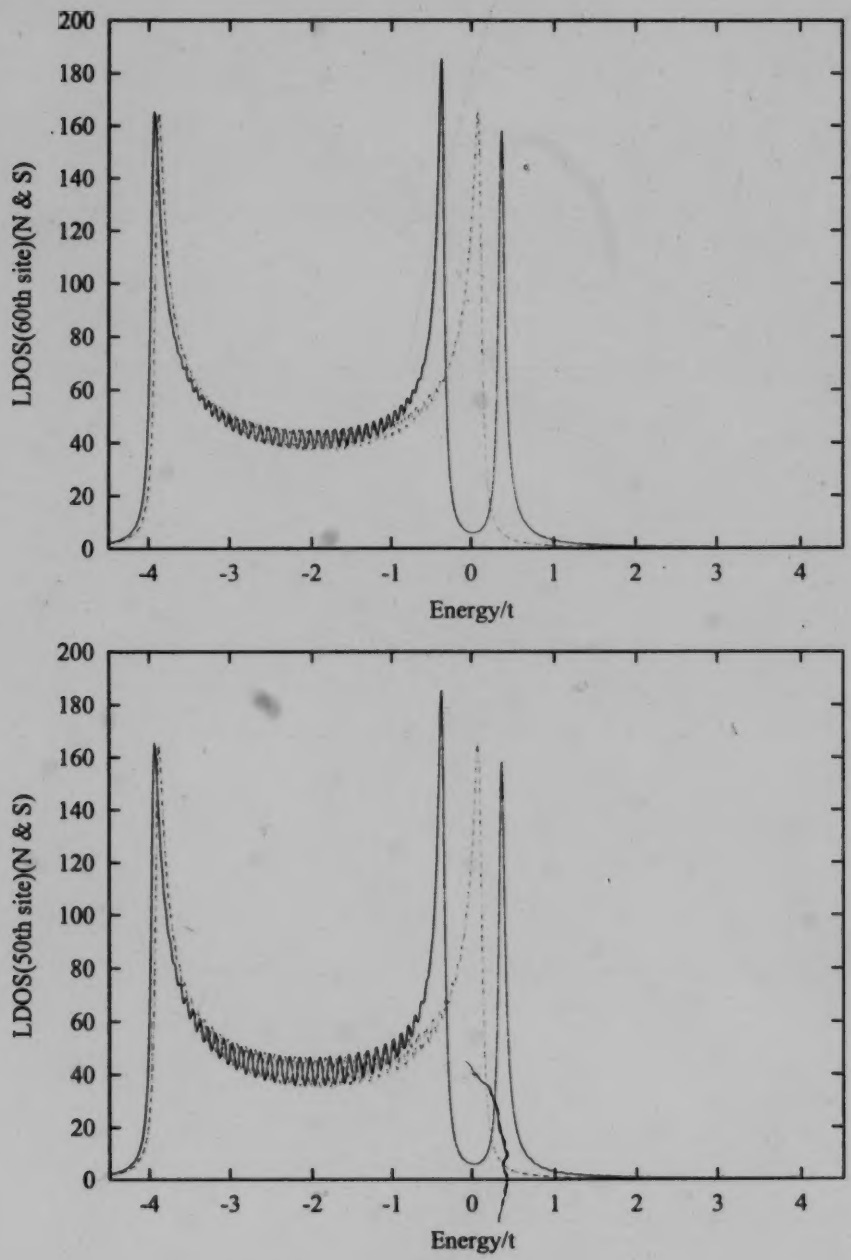

Figure 3.26: The same as FIG.(3.24) for 50th(down) and 60th(up) sites.

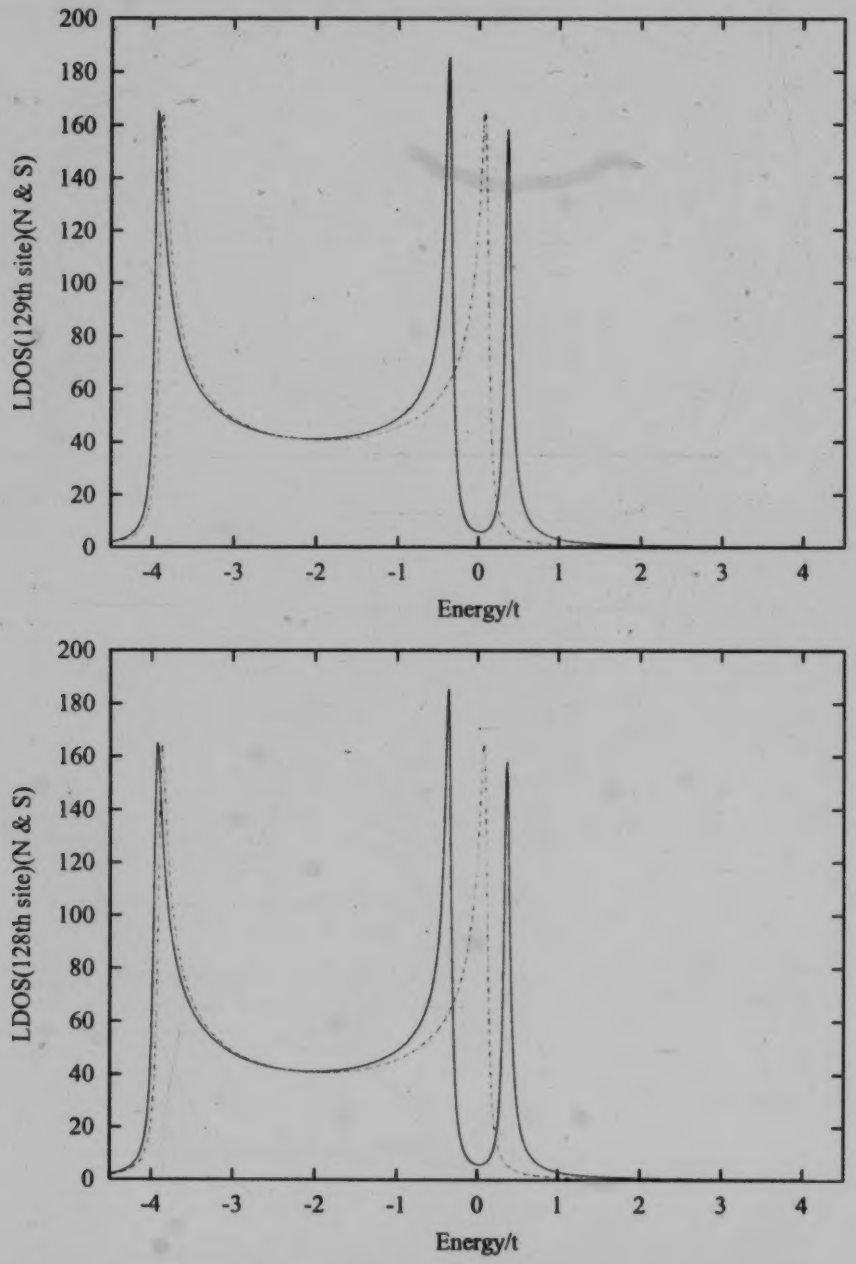

Figure 3.27: The same as FIG(3.24) for 128th(down) and 129th(up) sites. It is exactly the middle of system, and as can be seen the oscillations in LDOS almost vanish and we recover the BCS DOS.

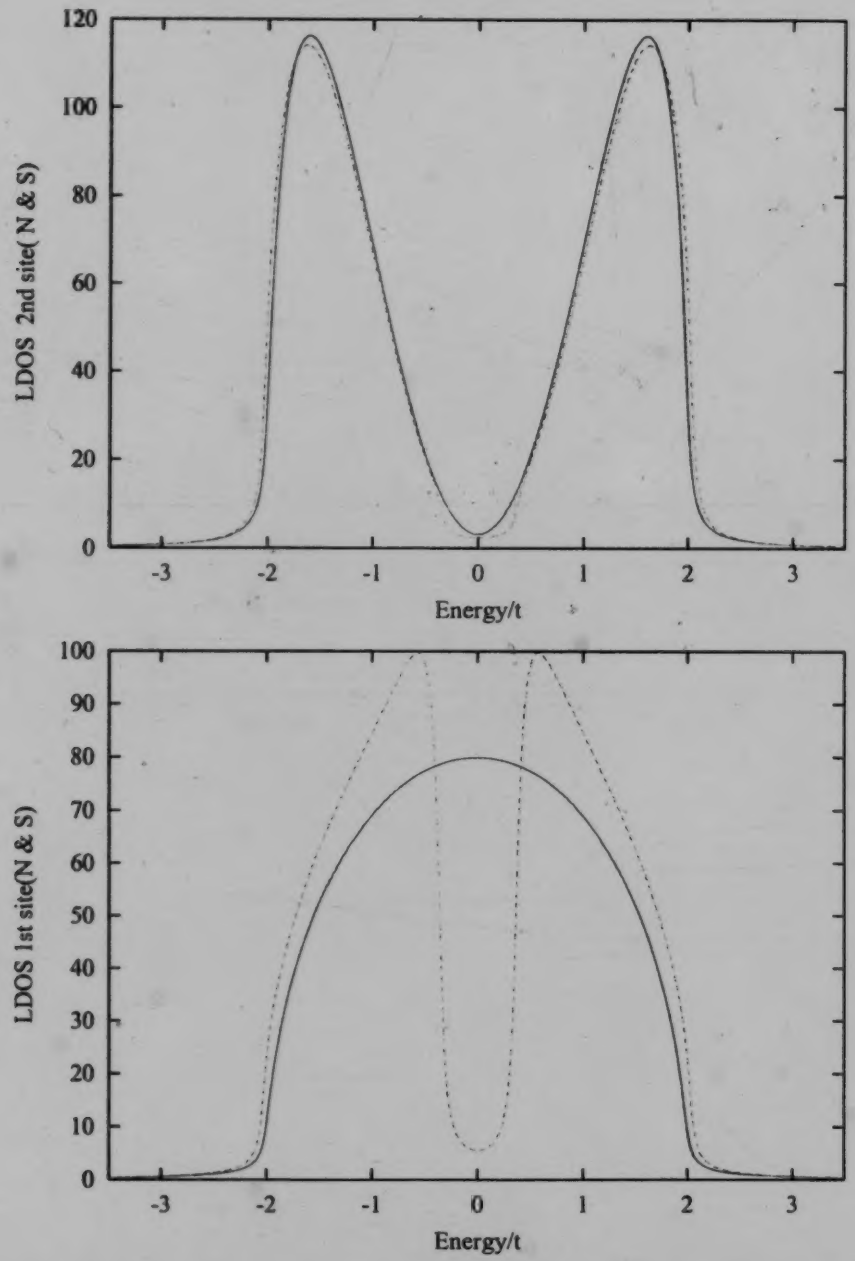

Figure 3.28: Local density of states(LDOS) for 256 site system at the first(down) and second(up) sites, at temperature ($T = 0.1t$), at a half-filling,$n_e = 1.0$, $|U| = 2.0t$. The solid lines are normal metal and dashed lines are superconducting solutions.

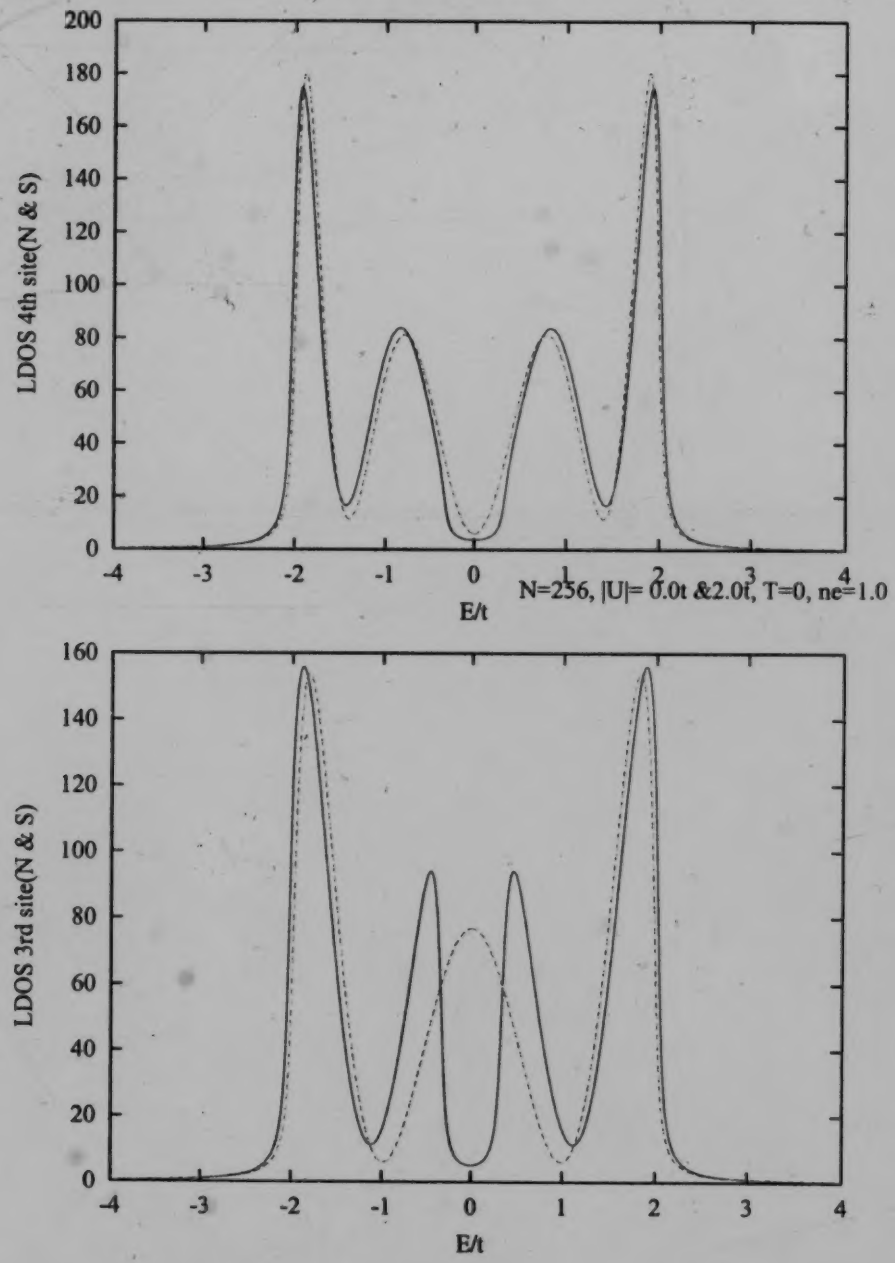

Figure 3.29: The same for as FIG(3.28)third(down) and fourth(up) sites.

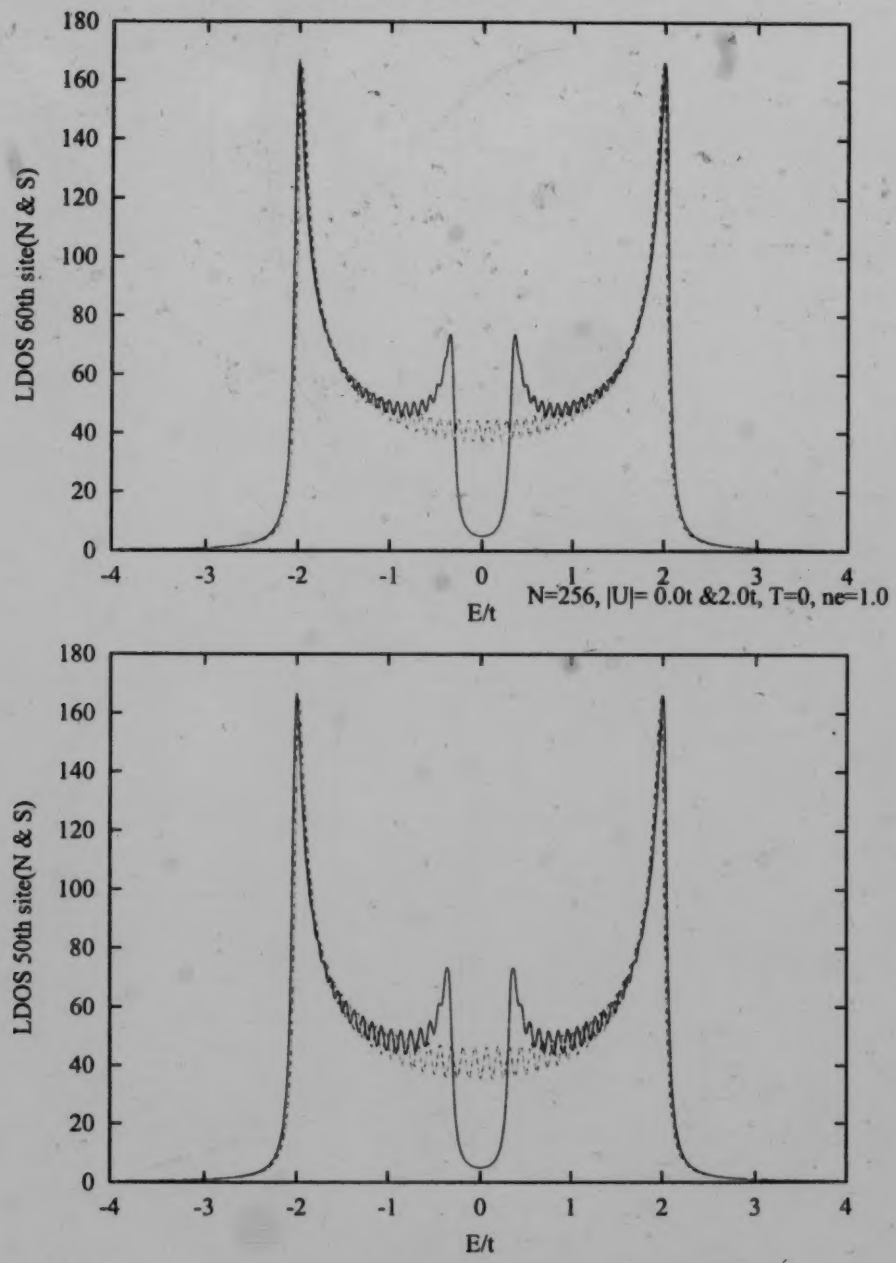

Figure 3.30: The same FIG(3.28)for 50th(down) and 60th(up) sites.

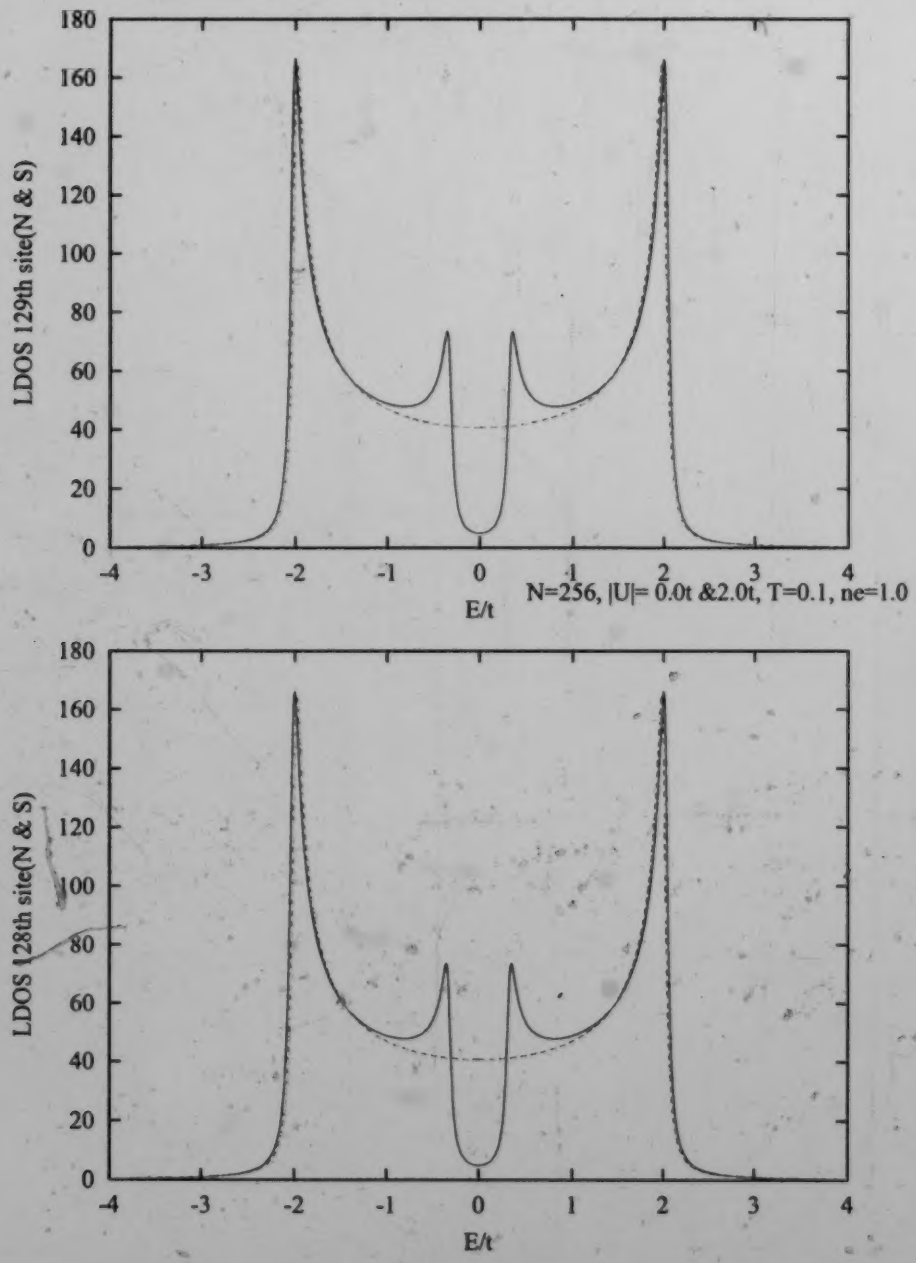

Figure 3.31: The same as FIG(3.28) for 128th(down) and 129th(up) sites. It is exactly the middle of system, and again as can be seen the oscillations in LDOS almost vanishes and we recover the BCS DOS form.

3.7.1 LDOS in the presence of a single impurity

From the experimental point of view, since there are recent STM experiments on both conventional and HTc superconductors that can give us the conductivity vs. voltage (that we know is proportional to the DOS of a superconductor) for a single impurity on the surface, the experiments are basically the surface density of states of our sample for a relevant range of energies. To check the theoretical justification for this we tried to check the LDOS of an impurity on the boundary. As already mentioned, this is also a check on whether an impurity on site + periodic boundary conditions can replace the tight-binding approximation that we used for our boundary conditions or not. Anyhow, the resulting DOS is interesting, since, especially near the impurity, on the second site ($V_{impurity} = 20t$) the density of states looks similar to Fig(3.20)(up), but with the little modification that one of the peaks in the LDOS is increased and the other is decreased (FIG. (3.32)-(3.33)) as we can see from tunneling experiments too [8]. It is actually obvious that this is a result of an impurity existing on the boundary, since we do not get any changes like this because of the surface. On our scale this difference is really fine, but it is also more likely to have stronger violations for d-wave superconductors as time reversal symmetry will be broken by the existence of the impurity [8].

Another important observation is that the LDOS on the first site does not look like the ones in the STM experiments, and the LDOS on the second site is more in agreement with the experiments. Introducing the impurity and observing that the heights of the peaks in the LDOS is changed as seen in STM experiments also suggests the idea that STM effectively probes the second site LDOS rather than first.

To check out all the other possible fine differences between an OBC model and PBC + impurity, I plotted the LDOS corresponding to sites far inside the

system (50th and 128th, FIGs(3.34)-(335)). In this region they look the same, as is actually expected since we might expect the same asymptotic behaviour for both boundary conditions.

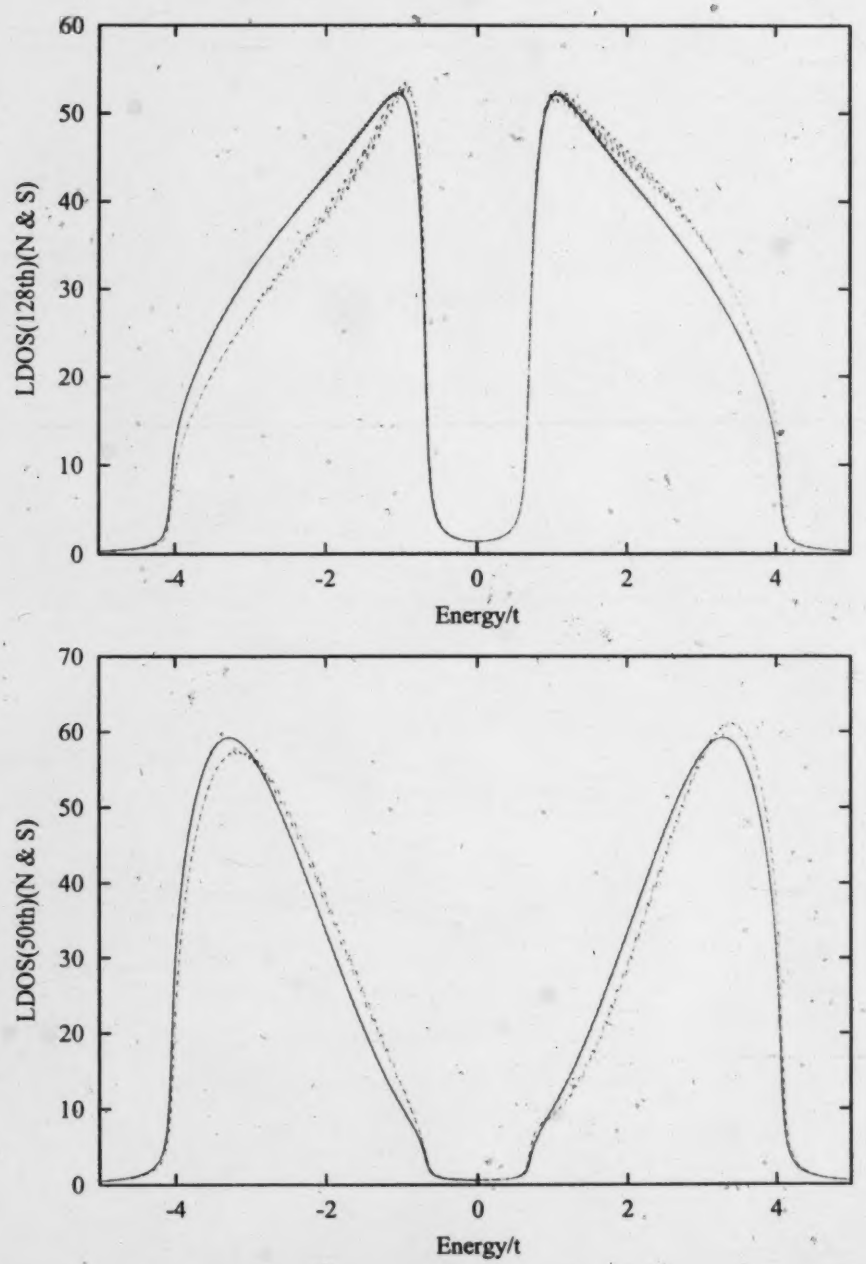

Figure 3.32: Local density of states(LDOS) for 256 site system at the first(up) and second(down) sites, at zero temperature($T = 0.01t$), $n_e = 1.0$ and $|U| = 2.0t$. The solid lines are PBC with non-magnetic impurity and dashed lines are solutions with OBC.

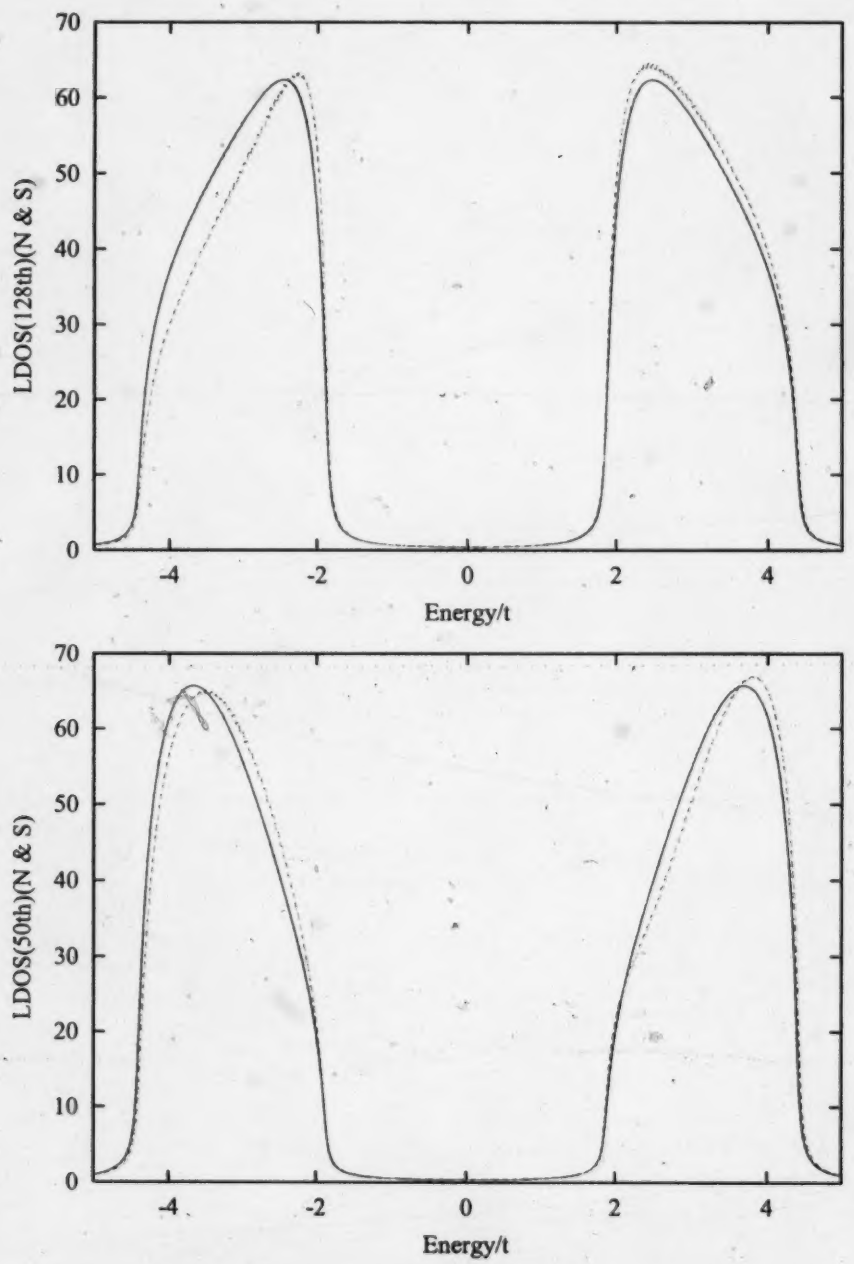

Figure 3.33: The same as FIG.(3.32) but with $|U| = 6t$

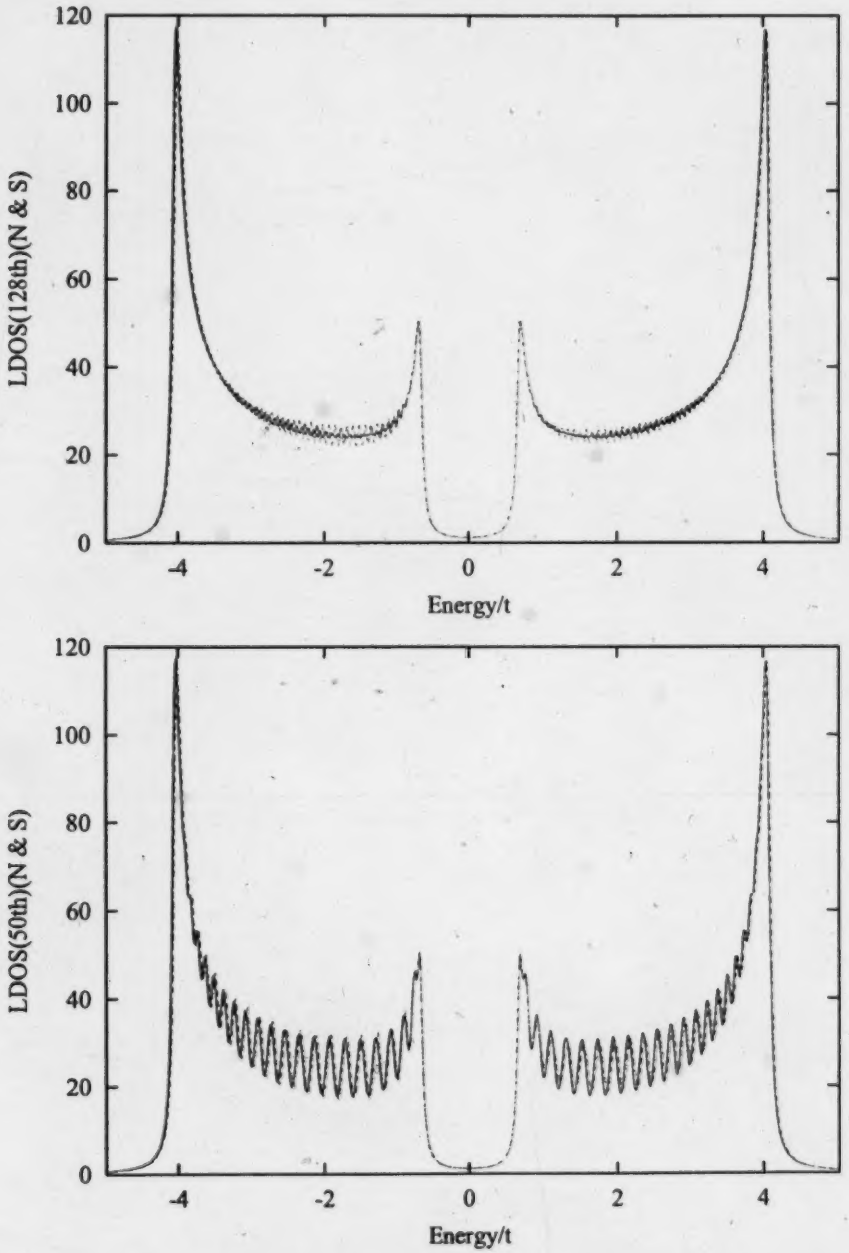

Figure 3.34: The same as FIG.(3.32 for 50th(down) and 128th(up) sites.

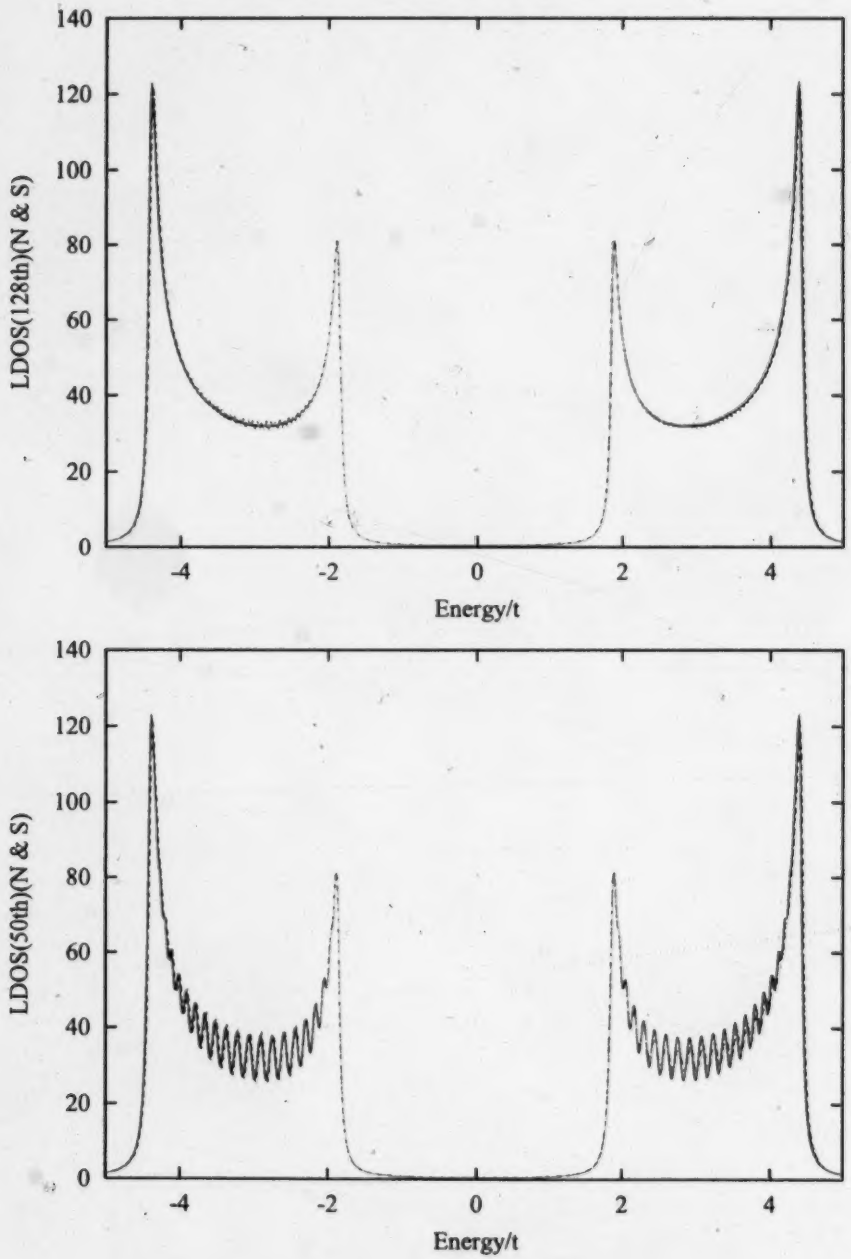

Figure 3.35: The same as FIG.(3.33) with $|U| = 6.0t$.

Conclusion

It can be seen that the self-consistent solutions of BdG obtained in the last chapter obviously show a contradiction with the quasi-classical approximation, although quasi-classical approximation is quite powerful in handling so many problems, specially because of its SUSY symmetry. Nonetheless, one of the objectives of this paper is to question the ability of the quasi-classical approximation for giving the right physical results on the microscopic level. The other result is the theoretical justification for the results obtained by Rowell et al [30] on the finite-size effects on the LDOS of a superconductor. Our result is in agreement with the previous work by Blaauboer et al [29] too. Still there are so many open problems for further study, such as comparison of the same behaviors for d-wave superconductors, and solving the problem for Josephson junctions, i.e., S-S or S-I-S junctions, rather than S-I that was our case of study. Moreover, the problem of rough surfaces is another interesting work to be considered, although this problem needs a lot of work and patience.

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